1972

A Numerical Study of Field-Aided Diffusion.

Ronald Quentin Perritt
Louisiana State University and Agricultural & Mechanical College

INFORMATION TO USERS

This dissertation was produced from a microfilm copy of the original document. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the original submitted.

The following explanation of techniques is provided to help you understand markings or patterns which may appear on this reproduction.

1. The sign or "target" for pages apparently lacking from the document photographed is "Missing Page(s)". If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting thru an image and duplicating adjacent pages to insure you complete continuity.

2. When an image on the film is obliterated with a large round black mark, it is an indication that the photographer suspected that the copy may have moved during exposure and thus cause a blurred image. You will find a good image of the page in the adjacent frame.

3. When a map, drawing or chart, etc., was part of the material being photographed the photographer followed a definite method in "sectioning" the material. It is customary to begin photoing at the upper left hand corner of a large sheet and to continue photoing from left to right in equal sections with a small overlap. If necessary, sectioning is continued again – beginning below the first row and continuing on until complete.

4. The majority of users indicate that the textual content is of greatest value, however, a somewhat higher quality reproduction could be made from "photographs" if essential to the understanding of the dissertation. Silver prints of "photographs" may be ordered at additional charge by writing the Order Department, giving the catalog number, title, author and specific pages you wish reproduced.

University Microfilms

300 North Zeeb Road
Ann Arbor, Michigan 48106

A Xerox Education Company

A NUMERICAL STUDY OF FIELD-AIDED DIFFUSION

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Electrical Engineering

by
Ronald Quentin Perritt
M.S., Louisiana State University, 1968
December, 1972

ACKNOWLEDGEMENT

The author wishes to express his most sincere appreciation to Dr. Alan H. Marshak for his valuable assistance in the preparation of this dissertation and for his friendship and guidance during the course of this research. He would also like to thank Dr. Leonard C. Adams for providing financial assistance over the past several years. Thanks also go to his many friends who have provided encouragement and assistance. In particular, he would like to thank Mrs. Debra Blanchard for typing the manuscript and his lovely wife Patsy for her constant support and encouragement.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

The object of this research is to ascertain the behavior of singly ionized impurity atoms diffusing in an initially intrinsic semiconductor. The effect of the internal electric field which arises during the diffusion process on the motion of the impurity ions is examined. The transport model defined by a system of non-linear equations describing the motion and interaction of the holes, electrons, and impurity ions is presented. Appropriate boundary conditions and initial values are discussed. An iteration technique for numerically solving the system of equations is described. Diffusion profiles are obtained for boron diffusing in silicon at $1100^{o}C$ for various values of surface concentration C_o. These profiles are compared to the complementary error function which is the correct solution neglecting the internal electric field. The effect of the field on the motion of the impurity ions is found to depend on C_o; as C_o is increased, the electric field enhances the diffusion of ions in the semiconductor. The impurity profiles are also compared to those obtained by solving an approximate diffusion equation. This approximate equation is derived using the concept of a concentration dependent "effective" diffusion coefficient. It is shown that the accuracy of the solutions obtained from solving the approximate diffusion equation depends on the value of C_o and the diffusion time. The errors increase with increasing C_o and diffusion time. Several recommendations are made for extending the basic numerical technique to other areas.

CHAPTER 1

INTRODUCTION

The term "diffusion," when applied in semiconductor device fabrication, is used loosely to describe the motion of impurity atoms at elevated temperatures within a semiconductor material. Diffusion under controlled conditions is employed in the manufacture of diodes, transistors, integrated circuits, and most other semiconductor devices. For example, a semiconductor material such as silicon is heated in a furnace to a temperature of around $1000^{\circ}C$. Impurity atoms are introduced into a flowing inert gas which deposits the impurity atoms on the surface of the semiconductor. Usually the gas deposits impurity atoms fast enough so that the concentration of impurity atoms on the surface is maintained at the solid solubility level. As the impurity atoms cross the surface and move into the semiconductor, most of them ionize. If the motion of these impurity ions were essentially the same as the diffusion of neutral particles, the flux f, or the number of ions crossing a unit area in unit time, is given by Fick's Law. For one-dimensional motion,

$$f = - D \frac{\partial c(x,t)}{\partial x}$$

where D is the diffusion constant and c(x,t) represents the concentration of ions or number of ions per unit volume. The ions also satisfy a continuity equation given by

$$\frac{\partial f}{\partial x} + \frac{\partial c}{\partial t} = 0$$

By using Fick's law for the flux in the above equation, we obtain

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \qquad (1\text{-}1)$$

which is called the simple diffusion equation. The solution to (1-1) for a semi-infinite solid, where $c(0,t)$ is constant and $c(x,0) = 0$ for $x > 0$, is given by the complementary error function,

$$c(x,t) = C_0 \operatorname{erfc}\left[x/(4Dt)^{1/2}\right]$$

$$c(x,t) = C_0 \operatorname{erfc}\left[x/(4Dt)^{1/2}\right]$$

where $C_0 = c(0,t)$ is the surface concentration.

It has been known for many years that this distribution does not agree with those obtained experimentally. One theory widely used to explain this disagreement is that an electic field arises during the diffusion process which enhances the motion of the impurity ions. This phenomenon is called field-aided diffusion. The field is produced by the separation of charge due to the ionization of the impurity atoms. For example, suppose boron atoms diffuse into a semiconductor. Because of the high temperature, the boron atoms ionize immediately producing negative ions and holes. The holes tend to diffuse away from the ions due to the much higher diffusion constant for holes. However, as the holes diffuse away, a space charge develops which produces an electric field. This field tends to retard the motion of the holes and enhance the motion of the ions.

The equations which govern the diffusion process are highly nonlinear and are discussed in section 1.1. There is no known analytical solution; however, several attempts have been made to simplify the equations so that approximate solution could be obtained to describe the effects of the electric field. A discussion of this work is presented in section 1.2. It is shown that there are serious inconsistencies in the assumptions made to simplify the diffusion equations which leave the results open to question.

In Chapter 2 a new approach to the study of field-aided diffusion is described. This approach is numerical and uses an iteration scheme to solve the basic equations. It does not employ the simplifying assumptions made in previous work. It is the first unified approach to the study of a singly ionized impurity species diffusing into an initially intrinsic material. Since planar technology, in which diffusion takes place primarily in only one direction, away from the surface, has become the principal method of fabricating semiconductor devices, the analysis is restricted to one-dimensional motion. The results of this new approach are presented in Chapter 3 and are compared with previous work. The conclusions are presented in Chapter 4.

1.1. The Transport Equations

In an intrinsic semiconductor, holes and conduction electrons are produced in equal numbers by thermal processes. When the temperature of the semiconductor is held fixed, the concentrations of holes and electrons are constant due to the simultaneous generation and recombination of hole-electron pairs. Now when impurity atoms are

introduced and subsequently ionize, the concentration of holes is altered, and because of recombination, the concentration of electrons will also be altered. Since the charge density at any point is a function of the concentration of holes, electrons and impurity ions, it is necessary to consider the motion of the electrons and holes as well as the motion of the impurity ions.

Treating the wafer as if it were semi-infinite, the model of the diffusion process for $x \geq 0$ and $t \geq 0$ is defined by the flux equations, the continuity equations and Gauss' Law. As stated earlier, the analysis is restricted to flow in one direction. Letting p, n and c represent the concentration of holes, electrons and impurity ions, respectively, the flux equations are given by

$$f_p = -D_p \frac{\partial p}{\partial x} + \mu_p pE \tag{1-2}$$

$$f_n = -D_n \frac{\partial n}{\partial x} - \mu_n nE \tag{1-3}$$

$$f_c = -D_c \frac{\partial c}{\partial x} + z\mu_c cE \tag{1-4}$$

where E is the electric field, D is the diffusion constant and μ is the mobility; $z = 1$ if c represents a donor impurity and $z = -1$ if c represents an acceptor impurity. The mobility and diffusion constant are related by the Einstein relation $D/\mu = kT/e = V_T$, where k is Boltzmann's constant, T is the temperature in degrees Kelvin and e is the electronic charge. The continuity equations for holes, electrons and impurity ions are given by

$$\frac{\partial p}{\partial t} = -\frac{\partial f_p}{\partial x} + G_p \tag{1-5}$$

$$\frac{\partial n}{\partial t} = - \frac{\partial f_n}{\partial x} + G_n \tag{1-6}$$

$$\frac{\partial c}{\partial t} = - \frac{\partial f_c}{\partial x} + G_c \tag{1-7}$$

where G_p, G_n and G_c represent the net generation rate of holes, electrons and impurity ions, respectively. Gauss' Law relates the electric field to the charge density ρ.

$$\frac{\partial E}{\partial x} = \frac{\rho}{\epsilon} = \frac{e}{\epsilon} (p - n + zc) \tag{1-8}$$

Since charge is conserved in the semiconductor, the particles must also satisfy the continuity relation

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0 \tag{1-9}$$

where J is the current density defined by

$$J = e(f_p - f_n + zf_c) \tag{1-10}$$

An auxiliary equation can be obtained by using (1-8) and (1-9) to give

$$\frac{\partial}{\partial x}\left(\epsilon \frac{\partial E}{\partial t}\right) + \frac{\partial J}{\partial x} = 0$$

or

$$\frac{\partial}{\partial x}\left(\epsilon \frac{\partial E}{\partial t} + J\right) = 0$$

This equation implies that

$$\epsilon \frac{\partial E}{\partial t} + J = K(t) \tag{1-11}$$

where in general K can be a function of time but not of position. Consider the diffusion of impurity atoms into a thick semiconductor wafer. Deep inside the material, far from the diffusing impurity atoms, the semiconductor is in thermal equilibrium so that E and J are zero there. Thus K is zero and (1-11) reduces to

$$\epsilon \frac{\partial E}{\partial t} + J = 0 \tag{1-12}$$

A relationship between the generation rates can easily be obtained by combining (1-8, 9 and 10) to give

$$\frac{\partial}{\partial t}(p - n + zc) + \frac{\partial f_p}{\partial x} - \frac{\partial f_n}{\partial x} + \frac{\partial f_c}{\partial x} = 0$$

By using (1-5), (1-6) and (1-7) we obtain

$$G_p - G_n + zG_c = 0$$

If we now assume that all impurity atoms are ionized at all times, then $G_c = 0$ and

$$G_p = G_n = G$$

We represent the net generation by the Schockly-Reed-Hall model given by

$$G = - \frac{pn - n_i^2}{\tau_n (p + n_i) + \tau_p (n + n_i)} \tag{1-13}$$

where n_i is the intrinsic concentration of electrons, τ_p and τ_n are the lifetimes of the holes and electrons respectively. The value of n_i depends strongly on the temperature at which the diffusion takes place.

There are several implicit assumptions which have been made thus far.

1. The permittivity of the material is constant.
2. The diffusion constants are independent of position and time.
3. The material is nondegenerate.
4. A one-dimensional analysis is adequate and the material can be treated as semi-infinite.
5. All impurity atoms are singly ionized at all times.

The number of equations describing the diffusion process can be reduced by substituting the flux equations into the continuity equations to give

$$\frac{\partial p}{\partial t} = D_p \left[\frac{\partial^2 p}{\partial x^2} - \frac{1}{V_T}\frac{\partial}{\partial x}(pE)\right] + G \qquad (1\text{-}14)$$

$$\frac{\partial n}{\partial t} = D_n \left[\frac{\partial^2 n}{\partial x^2} + \frac{1}{V_T}\frac{\partial}{\partial x}(nE)\right] + G \qquad (1\text{-}15)$$

and

$$\frac{\partial c}{\partial t} = D_c \left[\frac{\partial^2 c}{\partial x^2} - \frac{z}{V_T}\frac{\partial}{\partial x}(cE)\right] \qquad (1\text{-}16)$$

where the Einstein relation has been used. These three equations along with (1-8), (1-13) and (1-12) form the transport model for the

diffusion process. These equations represent three coupled, nonlinear, second order equations. Note that the nonlinearity is due to the fact that the electric field E is a function of p, n and c.

In the following section, a brief review is given of recent attempts to simplify this system of equations. Note that if the electric field were zero, (1-16) reduces to the simple diffusion equation (1-1).

1.2. Recent Work on Field-Aided Diffusion

It was pointed out by Zaromb [1] in 1957 and Smits [2] in 1958 that an electric field can arise during an isothermal diffusion process and that this field would act to enhance the motion of the impurity atoms. Zaromb considered the simultaneous diffusion of both donor and acceptor atoms and derived an approximate expression for the electric field in a semi-infinite material based on two major assumptions.

1. The material is charge neutral at every point so that

   $$\rho = p - n + zc = 0.$$

2. The product $pn = n_i^2$

Using (1-9) and assumption 1 it follows that J is independent of x. Thus since J = 0 deep inside the semiconductor, it must be zero everywhere. Now using (1-10) and the flux equations we have

$$-D_p \frac{\partial p}{\partial x} + D_n \frac{\partial n}{\partial x} - zD_c \frac{\partial c}{\partial x} + \frac{E}{V_T} (D_p p + D_n n + D_c c) = 0$$

and solving for E yields

$$E = V_T \frac{D_p \frac{\partial p}{\partial x} - D_n \frac{\partial n}{\partial x} + zD_c \frac{\partial c}{\partial x}}{D_p p + D_n n + D_c c} \tag{1-17}$$

Now using assumptions 1 and 2, p and n are given by

$$p = \frac{-zc + (c^2 + 4n_i^2)^{1/2}}{2}$$

$$n = \frac{zc + (c^2 + 4n_i^2)^{1/2}}{2}$$

Substituting these expressions into (1-17) and noting that at the elevated temperatures where diffusion of impurity atoms occurs, $D_c \ll D_n$, D_p, the electric field becomes

$$E = -z\, V_T \frac{\phi}{c} \frac{\partial c}{\partial x} \tag{1-18}$$

where $$\phi = \left[1 + \left(\frac{2n_i}{c}\right)^2\right]^{-1/2} \tag{1-19}$$

An expression similar to (1-18) was derived by Kurtz and Yee [3] even though they neglected the effect of the electron current. An effective diffusion constant D_c^* can be defined when (1-18) is used in the flux equation for the impurity atoms (1-4) to give

$$f_c = -D_c^* \frac{\partial c}{\partial x} \tag{1-20}$$

where $$D_c^* = D_c (1 + \phi) \tag{1-21}$$

Lehovec and Slobodskoy [4] substituted (1-20) into the continuity

equation (1-7) and assumed 100 percent ionization to obtain

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[D_c (1 + \phi) \frac{\partial c}{\partial x}\right] \qquad (1\text{-}22)$$

Approximate solutions were obtained for diffusion into intrinsic material. For strongly extrinsic material where $c \gg n_i$, $\phi \simeq 1$ from (1-19) and the effective diffusion constant $D_c^* \simeq 2D_c$. Shaw and Wells [5] considered the diffusion of singly ionized impurity atoms into a uniformly doped semiconductor using (1-22) as the model. Klein and Beal [6] considered the case of simultaneous diffusion of oppositely charged impurities by using an expression similar to (1-18) for the field. Their work was a generalization of Zaromb's work which was restricted to nearly intrinsic material.

All of the work on field-aided diffusion discussed thus far has been based on two key assumptions, $\rho = 0$ and $pn = n_i^2$. It follows from (1-8) that if $\rho = 0$, then $\partial E/\partial x = 0$ and E must be independent of x. Thus since E is zero deep inside the semiconductor, far from the diffusing impurity atoms, E must be zero everywhere. Obviously the field cannot be given by (1-18) and be zero simultaneously. Therefore the results obtained using (1-18) are open to question. Furthermore, there is little justification for the assumption that $pn = n_i^2$ other than it makes possible an analytical solution. The expression $pn = n_i^2$ is true only in thermal equilibrium and the error produced in using $pn = n_i^2$ when the semiconductor is out of thermal equilibrium cannot be determined.

In addition to making the above assumptions, Vas'Kin [7]

approximated the electric field by an average field arbitrarily defined in terms of a weighting function equal to the electron distribution. Bordina et al, [8] assumed for p and n the thermal equilibrium distributions. The only justification for such approaches appears to be that they permit an analytical solution.

It has been pointed out by Kennedy [9] that due to electrostatic shielding, the electric field given by (1-18) is probably much too large. His analysis, however, assumes the electron flux is zero and completely neglects the interaction of holes with electrons and impurity ions. His analysis is, therefore, incomplete.

There are other mechanisms which could effect the motion of impurity atoms. Thai [10] has discussed a process whereby dislocations in the semiconductor crystal can enhance the diffusion of impurities.

1.3. Problem Statement

The objective of this research is to ascertain the behavior of singly ionized impurity atoms diffusing into an initially intrinsic semiconductor under the influence of an internal electric field. The resulting profile c(x,t) will be compared with that obtained by solving the crude diffusion equation given by (1-22). It can then be determined under what conditions, if any, the simplified approach using (1-22) is valid.

The transport equations given by (1-14), (1-15), (1-16) and (1-12) constitute a system of three nonlinear, coupled equations in the three unknowns p, n and c. Since this system is intractable from an analytical viewpoint, the equations must be solved numerically.

The method used in an implicit iterative scheme and is described in detail in Chapter 2.

CHAPTER 2

METHOD OF SOLUTION

In Chapter 1 the partial differential equations which form the model for the diffusion of a singly ionized impurity species into a semiconductor material were presented. The purpose of this chapter is to describe an iterative method for numerically solving these equations for the case of a gaseous diffusion process in which the surface concentration of impurity atoms is maintained constant. The semiconductor is treated as semi-infinite in the x direction and is initially intrinsic.

The equations defining the model for the diffusion process are given by

$$\frac{\partial p}{\partial t} = D_p \left[\frac{\partial^2 p}{\partial x^2} - \frac{1}{V_T}\left(p \frac{\partial E}{\partial x} + E \frac{\partial p}{\partial x}\right)\right] + G \tag{2-1}$$

$$\frac{\partial n}{\partial t} = D_n \left[\frac{\partial^2 n}{\partial x^2} + \frac{1}{V_T}\left(n \frac{\partial E}{\partial x} + E \frac{\partial n}{\partial x}\right)\right] + G \tag{2-2}$$

$$\frac{\partial c}{\partial t} = D_c \left[\frac{\partial^2 c}{\partial x^2} - \frac{z}{V_T}\left(c \frac{\partial E}{\partial x} + E \frac{\partial c}{\partial x}\right)\right] \tag{2-3}$$

$$\frac{\partial E}{\partial x} = \frac{e}{\epsilon}\left(p - n + zc\right) \tag{2-4}$$

$$\frac{\partial E}{\partial t} = -\frac{e}{\epsilon}\left[-D_p \frac{\partial p}{\partial x} + D_n \frac{\partial n}{\partial x} - zD_c \frac{\partial c}{\partial x} + \left(D_p p + D_n n + zD_c c\right)\frac{E}{V_T}\right] \tag{2-5}$$

Before these equations can be solved, the boundary conditions and initial values must be specified. The surface concentration C_o of impurity atoms is constant and thus the boundary conditions at $x = 0$ are given in general by

$$\begin{aligned} c(0,t) &= C_o \ , \quad 0 \le t \le T \\ p(0,t) &= f(t) \\ n(0,t) &= f(t) \end{aligned}$$

where T is the maximum diffusion time and f(t) and g(t) are appropriate functions chosen in accordance with a model used to represent the dynamic processes occurring at the gas-solid interface defined by $x = 0$. There is no known way to determine f(t) and g(t) in general. The difficulty in finding appropriate boundary values to use at $x = 0$ is discussed in Appendix A; it is shown that the boundary conditions for holes and electrons at $x = 0$ can be approximated by

$$\begin{aligned} p(0,t) &= -\frac{z}{2} C_o + (C_o^2 + 4n_i^2)^{1/2} \\ n(0,t) &= n_i^2/p(0,t) \end{aligned} \tag{2-6}$$

where n_i is the intrinsic electron concentration evaluated at the diffusion temperature.

The semiconductor material is initially intrinsic and is assumed to be semi-infinite in the x direction. The hole and electron

concentrations at $x = \infty$ will not be affected by the injection of impurities at $x = 0$; thus the material at $x = \infty$ is in thermal equilibrium. Let L represent a numerical approximation to ∞. The boundary conditions at $x = L$ are

$$\begin{aligned} c(L,t) &= 0, \quad 0 \le t \le T \\ p(L,t) &= n_i \\ n(L,t) &= n_i \end{aligned} \tag{2-7}$$

The material is assumed to be initially intrinsic; thus the initial conditions at $t = 0$, prior to the diffusion of the impurity ions, are

$$\begin{aligned} p(x,0) &= n_i, \quad 0 < x < L \\ n(x,0) &= n_i \\ c(x,0) &= 0 \end{aligned} \tag{2-8}$$

The corresponding initial condition for the electric field is given by

$$E(x,0) = 0$$

This condition can be derived easily by integrating (2-4). Note that since the material is in thermal equilibrium at $x = L$, $E(L,t) = 0$, and by (2-8) the right-hand side of (2-4) is zero.

When these initial conditions are used in the numerical scheme described below, difficulties in the numerical accuracy arise due to the initially large time rate of change of c early in the diffusion process. These difficulties are discussed in Appendix B where it is shown that in order to avoid these problems, it is necessary to use

a set of starting conditions at some time $t > 0$. To start the iterative scheme, the following set of starting conditions is derived in Appendix B

$$c(x,t_o) = C_o \text{ erfc } \left[x/(4D_o t_o)^{1/2}\right] = \varphi(x)$$

$$p(x,t_o) = -\frac{z}{2}\varphi + \frac{1}{2}(\varphi^2 + 4n_i^2)^{1/2} \qquad (2\text{-}9)$$

$$n(x,t_o) = n_i^2/p(x,t_o)$$

$$E(x,t_o) = -zV_T \frac{1}{\varphi}\left[1 + \left(\frac{2n_i}{\varphi}\right)^2\right]^{-1/2} \frac{\partial\varphi}{\partial x}$$

where for convenience, $t_o = 120$ seconds.

2.1. Outline of the Iteration Scheme

The above equations completely define the diffusion process. The differential equations are nonlinear and coupled and have no known analytical solution. Thus it is necessary to use an approximation scheme in order to solve the diffusion problem. An implicit, iterative, numerical scheme was employed to solve this system of equations. This basic technique was successfully used by DeMari [11] to obtain the distributions of holes and electrons inside diodes operating at room temperature under transient conditions.

The iteration scheme is begun by calculating an approximate electric field at time $t_1 = t_o + \Delta t$ by using approximate distributions for p, n and c. This approximate field is then used to calculate

improved approximate distributions for p, n and c, from which an improved electric field is computed. This procedure is repeated until p, n and c satisfy an accuracy check; the program then proceeds to the next time step. The accuracy check used in the iterative procedure is discussed at the end of this section.

To illustrate how an approximate electric field is obtained consider (2-5) with $\partial E/\partial t$ represented by a forward difference formula at time $t_1 = t_0 + \Delta t$

$$\frac{E(x,t_1) - E(x,t_0)}{\Delta t} \simeq -\frac{e}{\epsilon}\left[-D_p \frac{\partial p(x,t_1)}{\partial x} + D_n \frac{\partial n(x,t_1)}{\partial x} - zD_c \frac{\partial c(x,t_1)}{\partial x}\right]$$

$$-\frac{e}{\epsilon}\left[D_p\, p(x,t_1) + D_n n(x,t_1) + D_c c(x,t_1)\right]\frac{E(x,t_1)}{V_T}$$

Solving for $E(x,t_1)$ gives

$$E(x,t_1) \simeq \frac{\dfrac{E(x,t_0)}{\Delta t} - \dfrac{e}{\epsilon}\left[-D_p \dfrac{\partial p}{\partial x} + D_n \dfrac{\partial n}{\partial x} - zD_c \dfrac{\partial c}{\partial x}\right]}{\dfrac{e}{V_T \epsilon}\left[D_p\, p + D_n n + D_c c\right] + \dfrac{1}{\Delta t}} \qquad (2\text{-}10)$$

where p, n, c and their derivatives are all evaluated at time t_1. Note that $E(x,t_0)$ is specified by the starting conditions. Now let $p^1(x,t_1)$, $n^1(x,t_1)$ and $c^1(x,t_1)$ be first approximations for p, n and c at time t_1 respectively. These first approximations could be based on an intuitive guess or simply set equal to the starting distributions at $t = t_0$. Once these approximate distributions have been specified, their partial derivatives are computed using finite

difference methods and (2-10) is used to obtain a first approximation to the electric field denoted by $E^1(x,t_1)$.

Now to show how these approximate distributions are used to calculate improved distributions, consider the hole distribution $p^1(x,t_1)$. Let the second approximation $p^2(x,t_1)$ be defined by

$$p^2(x,t_1) = p^1(x,t_1) + \Delta p^2(x,t_1)$$

In general, the j + 1 approximation is given by

$$p^{j+1}(x,t_1) = p^j(x,t_1) + \Delta p^{j+1}(x,t_1) \ , \quad j = 1, 2, 3, \cdots \qquad (2\text{-}11)$$

where $\Delta p^{j+1}(x,t_1)$ is found using (2-1). Applying a forward difference formula to the left-hand side of (2-1) yields

$$\left.\frac{\partial p}{\partial t}\right|_{t_1} \simeq \frac{p(x,t_1) - p(x,t_0)}{\Delta t}$$

When $p(x,t_1)$ is approximated using (2-11), the above equation becomes

$$\left.\frac{\partial p}{\partial t}\right|_{t_1} \simeq \frac{p^j(x,t_1) + \Delta p^{j+1}(x,t_1) - p(x,t_0)}{\Delta t} \qquad (2\text{-}12)$$

Now using (2-12) for the left-hand side of (2-1) and substituting (2-11) for p in all terms on the right-hand side of (2-1) except the last term G, the following differential equation is obtained

$$\frac{\partial^2 \Delta p^{j+1}}{\partial x^2} - \frac{E^j}{V_T} \frac{\partial \Delta p^{j+1}}{\partial x} - f_{1p} \Delta p^{j+1} - \frac{e}{\epsilon V_T} \left[\Delta p^{j+1} \right]^2 = f_{2p} \qquad (2\text{-}13)$$

where

$$f_{1p} = \frac{1}{D_p \Delta t} + \frac{e}{\epsilon} \frac{1}{V_T} \left(2p^j - n^j + zc^j \right)$$

$$f_{2p} = - \frac{\partial^2 p^j}{\partial x} + \frac{E^j}{V_T} \frac{\partial p^j}{\partial x} + \frac{e}{\epsilon} \frac{1}{V_T} \left(p^j - n^j + zc^j \right) p^j$$

$$+ \frac{1}{D_p \Delta t} \left[p^j - p(x, t_o) \right] - \frac{G(p^j, n^j)}{D_p}$$

and $E^j(x,t_1)$ is the approximate electric field computed from (2-10) using p^j, n^j and c^j. If (2-11) were used in the G term of (2-1) the resulting differential equation for Δp^{j+1} would not have the simple form of (2-13), and would be considerably more difficult to solve. The slight inconsistency in evaluating G using p^j instead of p^{j+1} is not significant, however, since assuming the system converges, $\Delta p \rightarrow o$ and thus G will not be a strong function of Δp.

Consider the case where $j = 1$; f_{1p} and f_{2p} can be calculated since p^1, n^1 and c^1 has been specified and E^1 can be determined from (2-10). Thus (2-13) can be solved by any conventional means for the values $\Delta p^2(x,t_1)$. The technique used to solve (2-13) is discussed in detail in section 2.3. Once the values of $\Delta p^2(x,t_1)$ are known, (2-11) is used to obtain an improved approximation $p^2(x,t_1)$ to the hole distribution. An analagous scheme is used to compute $n^2(x,t_1)$ and $c^2(x,t_1)$ where

$$n^{j+1}(x,t_1) = n^{j}(x,t_1) + \Delta n^{j+1}(x,t_1) \qquad (2\text{-}14)$$

$$c^{j+1}(x,t_1) = c^{j}(x,t_1) + \Delta c^{j+1}(x,t_1) \qquad (2\text{-}15)$$

These improved distributions for p, n and c are now used in (2-10) to upgrade the electric field distribution. The iteration cycle is repeated and in the limit as j increases, $\Delta p^{j+1}(x,t_1)$, $\Delta n^{j+1}(x,t_1)$ and $\Delta c^{j+1}(x,t_1)$ approach 0 for all x. Thus the approximate distributions $p^j(x,t_1)$, $n^j(x,t_1)$ and $c^j(x,t_1)$ approach the exact distributions $p(x,t_1)$, $n(x,t_1)$ and $c(x,t_1)$ which satisfy the diffusion model defined by (2-1)-(2-5) at time t_1. These final distributions now form the starting conditions for the next time $t_2 = t_1 + \Delta t$. The program proceeds in this manner from the starting time t_0 through as many time steps as desired.

The number of iterations, and thus the amount of computer time required to complete one time step, is related to the desired accuracy of p, n and c. Therefore it is necessary to have a practical test for accuracy to ensure that p^j converges to p. The criterion used was that $\Delta p^{j+1}(x_i,t_k)$, $\Delta n^{j+1}(x_i,t_k)$ and $\Delta c^{j+1}(x_i,t_k)$ be less than 0.01% of $p^j(x_i,t_k)$, $n^j(x_i,t_k)$ and $c^j(x_i,t_k)$, respectively, for all i at any t_k.

The details of the numerical scheme are given in sections 2.2, 2.3 and 2.4. Figure 2.1 shows a block diagram which summarizes the iterative procedure.

2.2. Normalization of the Transport Equations

The equations which form the mathematical model of the diffusion process can be handled most conveniently in a computer program when

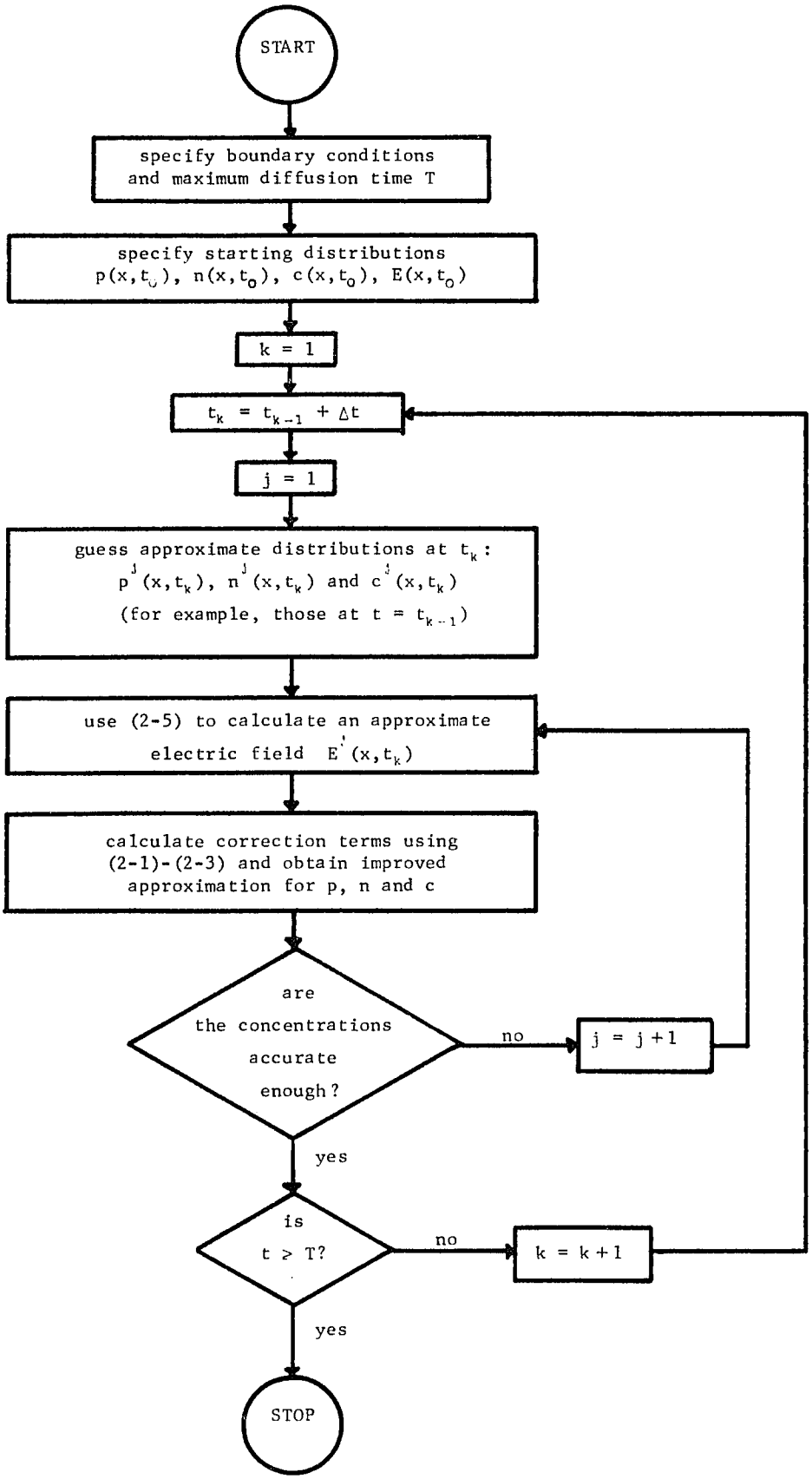

FIGURE 2.1. Block Diagram of the Iterative Procedure

they are written in dimensionless form. Table 2-1 gives the normalization factor for each quantity of interest; for example, the normalized hole concentration $\hat{p}$ is defined by $\hat{p} = p/n_1$. In order to keep the notation as simple as possible, no special symbols will be used to denote normalized quantities; all equations using normalized quantities will be explicitly identified. In terms of the normalized variables, the transport equations are

$$\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} - D_p (p - n + zc)p - D_p E \frac{\partial p}{\partial x} + G \tag{2-16}$$

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + D_n (p - n + zc)n + D_n E \frac{\partial n}{\partial x} + G \tag{2-17}$$

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2} - zD_c (p - n + zc)c - zD_c E \frac{\partial c}{\partial x} \tag{2-18}$$

$$\frac{\partial E}{\partial t} = D_p \frac{\partial p}{\partial x} - D_n \frac{\partial n}{\partial x} - zD_c \frac{\partial c}{\partial x} + (D_p p + D_n n + zD_c c)E \tag{2-19}$$

where

$$G = \frac{(pn - n_i^2/n_1^2)}{\tau_n (p + n_i/n_1) + \tau_p (n + n_1/n_1)}$$

2.3. Selection of Δt, Δx and L

The solution of the transport equations involves approximating partial derivatives with respect to x and t by finite differences. Thus it is necessary to select values of Δx and Δt which minimize the error introduced by these approximations. In order to determine approximate values of Δx and Δt, suitable for use in solving the transport

Quantity	Normalized Quantity	Normalization Factor
Particle Concentrations	p, n, c	n_1
Diffusion Constants	D_p, D_n, D_c	$D = 1cm^2/sec$
Position Coordinate*	x	$L_D = (\epsilon V_T/en_1)^{1/2}$
Time Coordinate	t	L_D^2/D
Lifetimes	τ_n, τ_p	L_D^2/D
Current Densities	J_p, J_n, J_c	en_1/L_D^2
Electric Field	E	V_T/L_D

*If the position coordinate is specified in microns, the normalization factor must be multiplied by 10^4.

TABLE 2-1: Normalization Factors for Quantities of Interest

equations, a computer program was written to solve the simple diffusion equation given by (1-1). Note that (2-3) reduces to (1-1) when the electric field is zero. The numerical solutions obtained using various combinations of Δx and Δt were then compared to the analytical solutions, given by the complementary error function, to determine the effects of Δx and Δt on the accuracy of the numerical solutions.

It was found that the accuracy was relatively independent of Δx for values of Δx between 0.01μ and 0.001μ. A nonuniform Δx was not found to have any advantage over a uniform Δx. It had the distinct disadvantage of requiring more computer time due to the increased number of calculations; therefore, a uniform Δx was selected.

The accuracy was found to decrease rapidly when values of $\Delta t > 0.5$ seconds were used. A $\Delta t = 0.1$ seconds provided only a slight improvement in accuracy over that obtained for $\Delta t = 0.5$ sec. Since the amount of computer time required to obtain a solution increased as Δt decreased, a compromise between accuracy and computer time must be made. Acceptable values of Δt were found to be in the range 0.1 to 0.5 seconds.

Using a $\Delta x = 0.004\mu$ or 0.005μ and $\Delta t = 0.5$ seconds, errors at the end of 60 seconds ranged typically from 0.01% close to the surface to 10% at a point where $c(x,t) = 10^{-7}C_o$. Larger errors occurred for smaller concentrations; however, because of the iterative nature of the technique, the errors were not cumulative. In fact the errors were found to decrease as t increased.

The method used to solve the above simple diffusion equation was exactly the same as outlined in section 2.1. The starting time

t_o and final time T were chosen to be 2 minutes and 30 minutes, respectively, the same as those used in the solution of the transport equations. The starting distribution $c(x,t_o)$ was given by the complementary error function at 2 minutes.

Using the procedure discussed in conjunction with (2-7) the boundary condition at $x = \infty$ is given by

$$c(L,\ t) = 0$$

where $x = L$ is the numerical approximation to $x = \infty$. The value of L must be chosen large enough so that as $x \rightarrow L$, $c(x,t) \rightarrow 0$ for all $t \leq T$. Note that the selection of L depends on the maximum diffusion time. A test to determine the proper value of L is to vary L and examine the effect on the distribution. The values of $c(x,t)$ must not be significantly influenced by changing L. A value of $L = 2\mu$ was found to be adequate for T = 30 minutes.

The above values of Δx, L and Δt were then used to obtain solutions of the transport equations as described in section 2.1. Choosing values of Δx and Δt based on the analysis of the solution to the simplified diffusion equation does not guarantee that these are the optimum choices for the solution to the system of nonlinear equations. It was found, however, that the solution to the system of nonlinear equations was not strongly dependent on Δx. It was also found that there was no significant difference between solutions obtained using a Δt of 0.5 seconds and those obtained using $\Delta t = 0.1$ seconds. This indicated that the solution was not a strong function of the choice of Δx and Δt, within the range of the values tested.

A check was made to determine the accuracy with which the iterative technique could solve the system of nonlinear equations. Consider the case where the surface concentration of impurity ions $C_O = 0.1n_i$. Since the number of particles introduced by the ionization of the impurities is at least one order of magnitude below the intrinsic values, it is reasonable to assume that the hole and electron concentrations would not be very different from n_i. Thus the assumptions of thermal equilibrium and charge neutrality are more nearly correct than for the case of higher impurity concentrations. Therefore the electric field should be small. An approximate diffusion equation was derived in Chapter 1 based on the above assumptions and is given by (1-22). The solution to (1-22) for $C_O = 0.1n_i$ is almost identical to the complementary error function. When the system of nonlinear equations was solved with $C_O = 0.1n_i$, the solution was also found to be almost identical to the complementary error function. Therefore it was concluded that the numerical technique for solving the system of nonlinear equations gives accurate results for the case of $C_O = 0.1n_i$. The results for this and higher values of C_O are presented in Chapter 3. In view of the high degree of accuracy observed in this special case, the results obtained for larger values of C_O can be viewed with confidence.

2.4. Determination of the Correction Terms

The equation which must be solved at each iteration in order to determine the correction terms is given by (2.13), and is repeated here in normalized form for convenience

$$\frac{\partial^2 \Delta p^{j+1}}{\partial x^2} - E^j \frac{\partial \Delta p^{j+1}}{\partial x} + f_{1p} \Delta p^{j+1} - \left[\Delta p^{j+1}\right]^2 = f_{2p} \tag{2-20}$$

where E^j, f_{1p} and f_{2p} are known functions as described in section 2.1. The corresponding normalized functions at time t_k are

$$f_{1p} = -\left[\frac{1}{D_p \Delta t} + (2p^j - n^j + zc^j)\right]$$

$$f_{2p} = -\frac{\partial^2 p^j}{\partial x^2} + E^j \frac{\partial p^j}{\partial x} + (p^j - n^j + zc^j)p^j \tag{2-21}$$

$$+ \frac{1}{D_p \Delta t}\left[p^j - p(x, t_k - \Delta t)\right] - \frac{G(p^j, n^j)}{D_p}$$

and the boundary conditions are

$$\Delta p^j(0, t_k) = \Delta p^j(L, t_k) = 0 \ , \quad \text{all } j \text{ and } k \tag{2-22}$$

The solution to (2-20) can be found by solving a system of algebraic equations obtained by approximating the derivatives in (2-20) by the following finite difference formulas [12]

$$\left.\frac{\partial y(x, t_k)}{\partial x}\right|_{x_i} \simeq \frac{1}{2\Delta x}\left(y_{i+1} - y_{i-1}\right)$$

$$\left.\frac{\partial^2 y(x, t_k)}{\partial x^2}\right|_{x_i} \simeq \frac{1}{(\Delta x)^2}\left(y_{i-1} - 2y_i + y_{i+1}\right)$$

where $y_i = y(x_i, t_k)$. When these formulas are used in (2-20), the

following system of algebraic equations is obtained

$$A_{p\,i}\ \Delta p_{i-1}^{j+1} + B_{p\,i}\ \Delta p_i^{j+1} + C_{p\,i}\ \Delta p_{i+1}^{j+1} = F_{p\,i} \tag{2-23}$$

where $$\Delta p_1^{j+1} = \Delta p_N^{j+1} = 0, \quad \text{all } j \text{ and } k$$

$$A_{p\,i} = \frac{2}{\Delta x} + E_i^j$$

$$B_{p\,i} = -2\left[(p_i^j - n_i^j + zc_i^j) + p_i^j + \frac{1}{D_p \Delta t}\right]\Delta x - \frac{4}{\Delta x}$$

$$C_{p\,i} = \frac{2}{\Delta x} - E_i^j$$

$$F_{p\,i} = 2\Delta x f_{2p}\Big|_{x_i}$$

$$i = 2, 3, 4, \cdots, N-1$$

Note that $x_1 = o$, $x_N = L$ and that normalized quantities are used. In order to evaluate f_{2p} given in (2-21), the following difference formulas [12] should be used for improved accuracy.

$$\frac{\partial y(x,t_k)}{\partial x}\Big|_{x_i} \simeq \frac{1}{12\Delta x}\left(y_{i-2} - 8y_{i-1} + 8y_{i+1} - y_{i+2}\right)$$

$$\frac{\partial^2 y(x,t_k)}{\partial x^2}\Big|_{x_i} \simeq \frac{1}{12(\Delta x)^2}\left(-y_{i-2} + 16y_{i-1} - 30y_i + 16y_{i+1} - y_{i+2}\right)$$

It is not necessary to use these higher order formulas for the derivatives of Δp^{j+1} since Δp^{j+1} is being reduced to zero as p^{j+1} becomes more accurate.

Equation (2-23) can be written in the form

$$[T][\Delta p] = [F_p]$$

where

$$[\Delta p] = \begin{bmatrix} \Delta p_2^{j+1} \\ \Delta p_3^{j+1} \\ \Delta p_4^{j+1} \\ \vdots \\ \Delta p_{N-1}^{j+1} \end{bmatrix}, \quad [F_p] = \begin{bmatrix} F_{P2} \\ F_{P3} \\ F_{P4} \\ \vdots \\ F_{P(N-1)} \end{bmatrix}$$

and

$$[T] = \begin{bmatrix} B_{P2} & C_{P2} & 0 & 0 & \cdots & \cdots & \cdots \\ A_{P3} & B_{P3} & C_{P3} & 0 & \cdots & \cdots & \cdots \\ 0 & A_{P4} & B_{P4} & C_{P4} & 0 & \cdots & \cdots \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \cdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & & \ddots & \ddots & \ddots & C_{P(N-2)} \\ \vdots & \vdots & \cdots & 0 & A_{P(N-1)} & \cdots & B_{P(N-1)} \end{bmatrix}$$

A simple direct method [11] can be employed to solve this system of algebraic equations. Basically, the method consists of finding quantities g_m and h_m which satisfy the recursion relation

$$\Delta p_m^{j+1} = g_m - h_m \Delta p_{m+1}^{j+1} \qquad m = N-1, N-2, \cdots, 2 \qquad (2\text{-}24)$$

where $g_1 = h_1 = 0$ since $\Delta p_1^{j+1} = 0$, all j. Substitution of (2-24) with

with m = i-1 into (2-23) yields

$$g_i = \frac{F_{p\,i} - A_{p\,i}\ g_{i-1}}{B_{p\,i} - A_{p\,i}\ h_{i-1}}$$

and

$$h_i = \frac{C_{p\,i}}{B_{p\,i} - A_{p\,i}\ h_{i-1}}$$

where $i = 2,3, \cdots, N-1$

After the correction terms Δp_i^{j+1} have been calculated, a better approximation to the hole distribution is obtained by using a discrete version of (2-11); thus

$$p_i^{j+1} = p_i^{j} + \Delta p_i^{j+1}$$

The procedure for obtaining Δn^{j+1} is entirely analagous to that used to find Δp^{j+1}. The improved hole distribution is now used to calculate the correction terms for the electron distribution. The normalized equations required to determine Δn^{j+1} at time t_k, are

$$A_{n\,i}\Delta n_{i-1}^{j+1} + B_{n\,i}\Delta n_i^{j+1} + C_{n\,i}\Delta n_{i+1}^{j+1} = F_{n\,i} \qquad (2\text{-}25)$$

where

$$\Delta n_1^{j+1} = \Delta n_N^{j+1} = 0, \text{ all } j \text{ and } k$$

$$A_{n\,i} = \frac{2}{\Delta x} - E_i^j$$

$$B_{n\,i} = 2\left[\left(p_i^{j+1} - n_i^j + zc_i^j\right) - n_i^j - \frac{1}{D_n \Delta t}\right]\Delta x - \frac{4}{\Delta x}$$

$$C_{n\,i} = \frac{2}{\Delta x} + E_i^j$$

$$F_{n\,i} = 2\Delta x\left[-\left(\frac{\partial^2 n^j}{\partial x^2}\right)_i - E_i^j\left(\frac{\partial n^j}{\partial x}\right)_i\right.$$

$$\left. - \left(p_i^{j+1} - n_i^j + zc_i^j\right) n_i^j\right]$$

$$+ \frac{2\Delta x}{D_n \Delta t}\left[n_i^j - n(x_i,\ t_k - \Delta t)\right] - \frac{2\Delta x G_i\,(p^{j+1},\ n^j)}{D_n}$$

$$i = 2,\ 3,\ 4,\ \cdots\ N-1$$

The method of solution of (2-25) is the same as that used to solve (2-23). The improved electron distribution is then computed using

$$n_i^{j+1} = n_i^j + \Delta n_i^{j+1}$$

This new electron distribution, along with p_i^{j+1}, is now used in the calculations to determine Δc_i^{j+1}. The appropriate normalized equations at time t_k are given by

$$A_{c\,i}\Delta c_{i-1}^{j+1} + B_{c\,i}\Delta c_i^{j+1} + C_{c\,i}\Delta c_{i+1}^{j+1} = F_{c\,i} \qquad (2\text{-}26)$$

where $\Delta c_1^{j+1} = \Delta c_N^{j+1} = 0$, all j and k

$$A_{c\,i} = \frac{2}{\Delta x} + z\,E_i^j$$

$$B_{c\,i} = -2\left[z\left(p_i^{j+1} - n_i^{j+1} + zc_i^j\right) + c_i^j + \frac{1}{D_c \Delta t}\right]\Delta x - \frac{4}{\Delta x}$$

$$C_{c\,i} = \frac{2}{\Delta x} - z\,E_i^j$$

$$F_{c\,i} = 2\Delta x\left[-\left(\frac{\partial^2 c^j}{\partial x^2}\right)_i + z\,E_i^{j+1}\left(\frac{\partial c^j}{\partial x}\right)_i\right.$$

$$\left. + z\left(p_i^{j+1} - n_i^{j+1} + zc_i^j\right)c_i^j\right] +$$

$$\frac{2\Delta x}{D_c \Delta t}\left[c_i^j - c\left(x_i,\ t_k - \Delta t\right)\right]$$

$$i = 2,\ 3,\ 4,\ \cdots\ N-1$$

The solution to (2-26) is analogous to the solution to (2-23) and (2-25). The improved impurity ion distribution can now be found using

$$c_i^{j+1} = c_i^j + \Delta c_i^{j+1}$$

After the approximate distributions for p, n and c have been upgraded, an improved electric field is computed from (2-10) and the cycle is repeated until the particle distributions have satisfied the accuracy check. Then t is incremented by Δt and the iteration procedure is begun again.

This numerical procedure was used to obtain the impurity ion

distributions for the case of boron diffusing in silicon at 1100^{o}C. The results are presented in Chapter 3. Also presented are the distributions obtained using (1-22) which was derived based on several assumptions. These simplifying assumptions allowed an approximate electric field to be found analytically.

CHAPTER 3

NUMERICAL RESULTS

The purpose of this chapter is to describe the behavior of singly ionized atoms diffusing in initially intrinsic material. The surface concentration of impurity atoms was maintained constant using a gaseous diffusion process. The numerical computation was executed on an IBM S/360 computer; the program listing and user's guide are given in Appendix C. The program determined the impurity ion distributions $c(x,t)$ for $0 < x < 2\mu$ and $2 \leq t \leq 30$ minutes using the method described in Chapter 2 with $\Delta x = 0.005\mu$ and $\Delta t = 0.5$ seconds. Presented here are the impurity profiles for $t = 2$, 10 and 30 minutes. The effect of the electric field on the motion of the impurity ions can be determined by comparing the numerical results to the complementary error function. The impurity distributions are then compared to those obtained by solving the approximate diffusion equation (1-22). It can then be determined under what conditions, if any, the use of (1-22) can be justified.

For convenience, boron is assumed to be diffusing in silicon at $1100^{\circ}C$. The intrinsic concentration of electrons at $1100^{\circ}C$ is approximately 10^{19} cm^{-3} [13]. The diffusion constants for holes and electrons at the diffusion temperature are given by [14]

$$D_n \simeq 6 \text{ cm}^2/\text{sec}$$

$$D_p \simeq 2 \text{ cm}^2/\text{sec}$$

The diffusion constant for boron ions [15] is

$$D_c \simeq 1.6 \times 10^{-13} \text{ cm}^2/\text{sec}$$

and since these ions are acceptors, z = -1.

Before the results are presented, it is necessary to discuss briefly the values used for the hole and electron lifetimes τ_p and τ_n. No data on the exact values of τ_n and τ_p applicable to the present study could be found. In order to determine the effect of τ_n and τ_p on c(x,t), the lifetimes were arbitrarily set equal and varied over the range 10^{-6} sec. to 5×10^{-11} sec.; c(x,t) was not found to be strongly dependent on the lifetimes. The values of $\tau_p = \tau_n = 10^{-9}$ sec. were used in the results presented below.

In order to illustrate the effect of the surface concentration C_o of impurity ion on the diffusion process, results were obtained for $C_o/n_i = \beta = 0.1$, 1, 10, 100 and 200. These values cover the typical range of values of C_o for boron.

The impurity profiles for the above values of β were obtained by solving the transport equations as described in Chapter 2; they are shown in Figures 3.1 through 3.5. Each figure shows the impurity profile for t = 2, 10 and 30 minutes. The curve at $t = t_o = 2$ minutes is obtained from

$$c(x,t) = C_o \text{ erfc } \left[x(4D_c t)^{-1/2} \right] \qquad (3\text{-}1)$$

Recall that t_o is the starting time. Also plotted are profiles corresponding to (3-1) evaluated at t = 10 and 30 minutes. These profiles correspond to the solutions when the electric field is zero. Note

that the quantity plotted along the vertical axis is c/n_i and that at $x = 0$, $c/n_i = C_o/n_i = \beta$.

From Figure 3.1 it can be seen that for $\beta = 0.1$, the impurity ion distributions at $t = 10$ and 30 minutes obtained by solving the transport equations are essentially the same as those given by (3-1). Thus it can be concluded that with a low surface concentration corresponding to $\beta \leq 0.1$, the electric field which arises during the diffusion process does not have a significant effect on the motion of the ions.

Figures 3.2 and 3.3 show that as the surface concentration is increased, the deviation between the numerical results obtained by solving the transport equations and the erfc increases. When $\beta = 1$ the impurity profile for $t = 30$ minutes is larger than the erfc by an average of approximately 30% over the region shown in Figure 3.2. When $\beta = 10$, the values of $c(x,t)$ at $t = 30$ minutes are approximately 5 times larger than the erfc for $0.5 < x < 0.75\mu$.

It can be seen from Figures 3.4 and 3.5 that when $C_o/n_i \geq 100$, the impurity profiles differ significantly from the complementary error function. Consider the case where $\beta = 100$. At $t = 30$ minutes, in the range $x \leq 0.75\mu$, the profile is linear when plotted on semilog paper; thus the impurity ion concentration is exponentially decreasing with x in this range. Figure 3.6 shows this profile in greater detail. The electric field is acting to greatly enhance the motion of the impurity ions. A close comparison of the curves of $t = 30$ minutes reveals that if the erfc curve were used to approximate the impurity profile, then for $x > 0.8\mu$, the values of c would be in error by more than one

order of magnitude.

The maximum value of the charge density $e(p - n + zc)$ was found to be on the order of 10^{-3} coul/cm^3. The ratio $|p - n + zc| /(p + n + c)$ gives a relative measure of charge neutrality. For $\beta = 10$, the maximum value of this ratio was approximately 10^{-4}. Since p, n and c can be expected to be accurate out to at least 3 decimal places, the charge density is approximately zero within the accuracy of the numerical technique.

It must not be inferred from the above discussion that because $\rho \simeq 0$ the electric field is approximately zero. The electric field is determined by using (2-5); thus the calculation of the field does not depend directly on the value of the net charge density.

For $\beta \geq 1$, the maximum value of the electric field occurred in the region where $c(x,t)$ was greater than or comparable to n_i. The maximum value of the field was found to be on the order of 10^4 v/cm and occured early in the diffusion process. In all cases, the maximum value of the field was found to decrease with time.

In order to illustrate the relationship between surface concentration and the effect of the electric field, consider the case of $\beta = 100$. At t = 30 minutes, the drift component of the impurity ion current density was $\geq$ 10% of the diffusion component for $0 \leq x \leq 0.9\mu$. When $\beta = 10$, the above condition was satisfied only for $0 \leq x \leq 0.7\mu$. When $\beta = 1$, the range was $0 \leq x \leq 0.35\mu$. The diffusion component was larger than the drift component in all cases. Thus it can be seen that the effect of the electric field on the motion of the impurity ions increases as the surface concentration is increased.

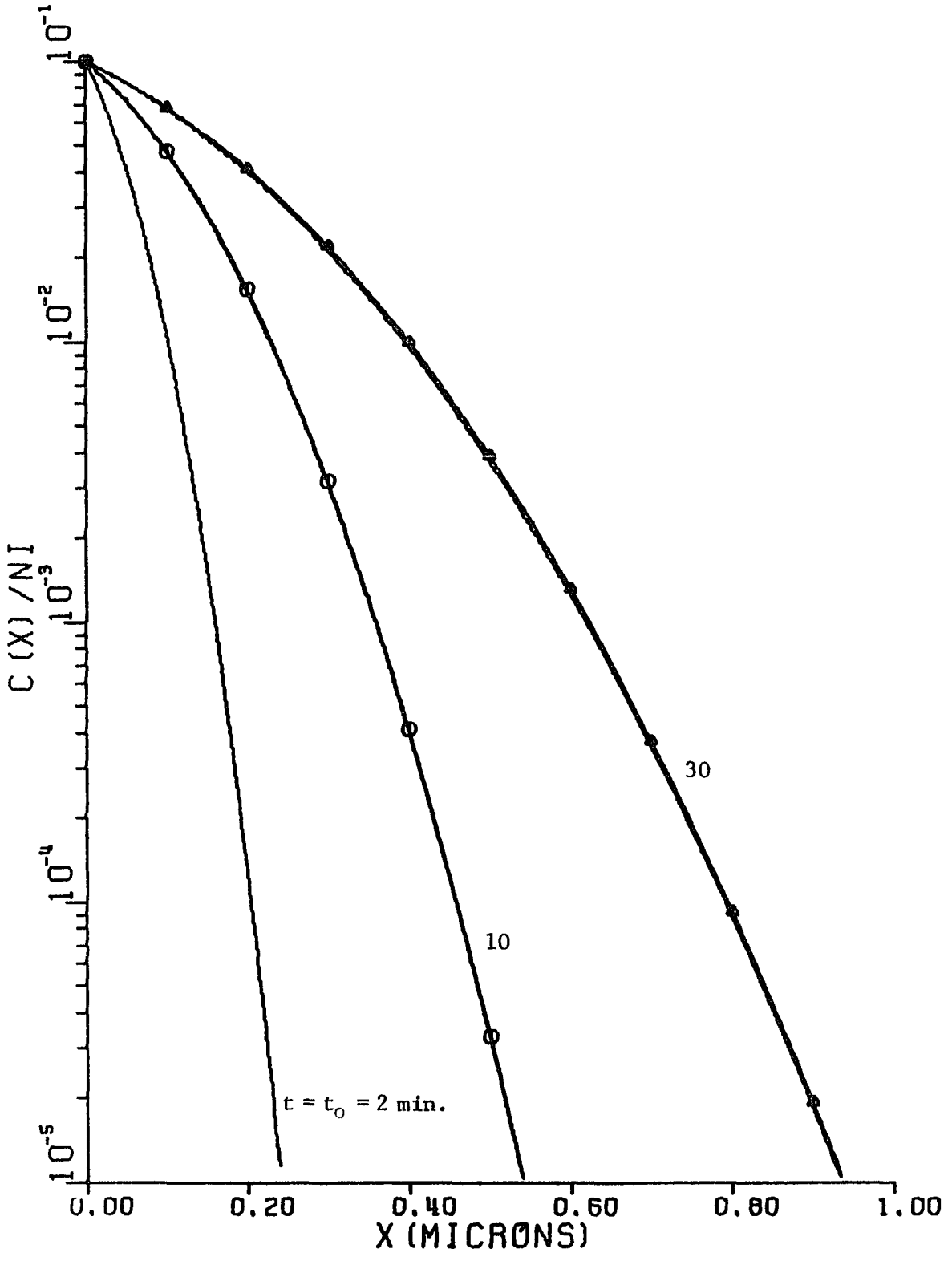

FIGURE 3.1. Impurity profiles for $\beta = 0.1$; unmarked curves represent the profiles when the field is zero.

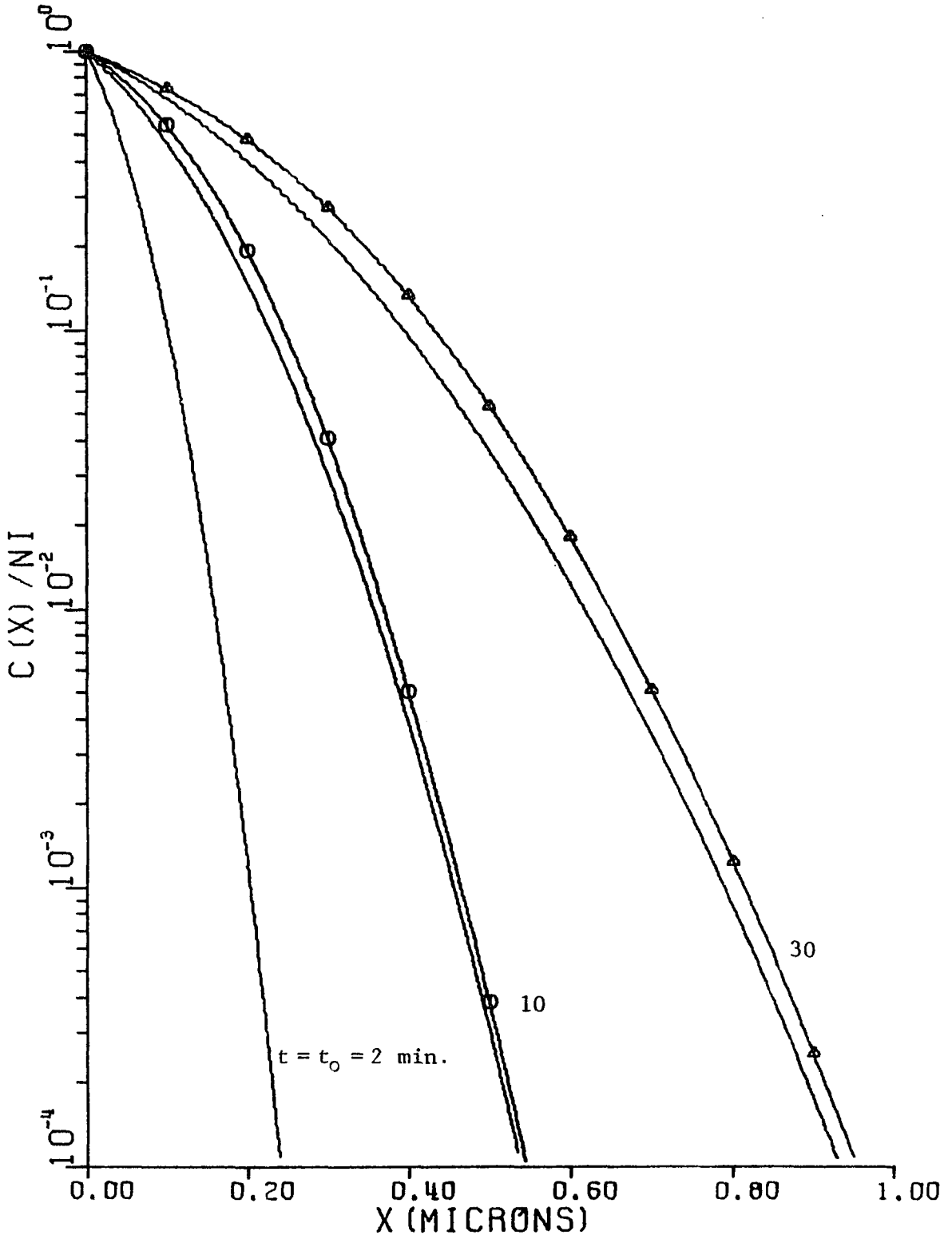

FIGURE 3.2. Impurity profiles for $\beta = 1$; unmarked curves represent profiles when the field is zero.

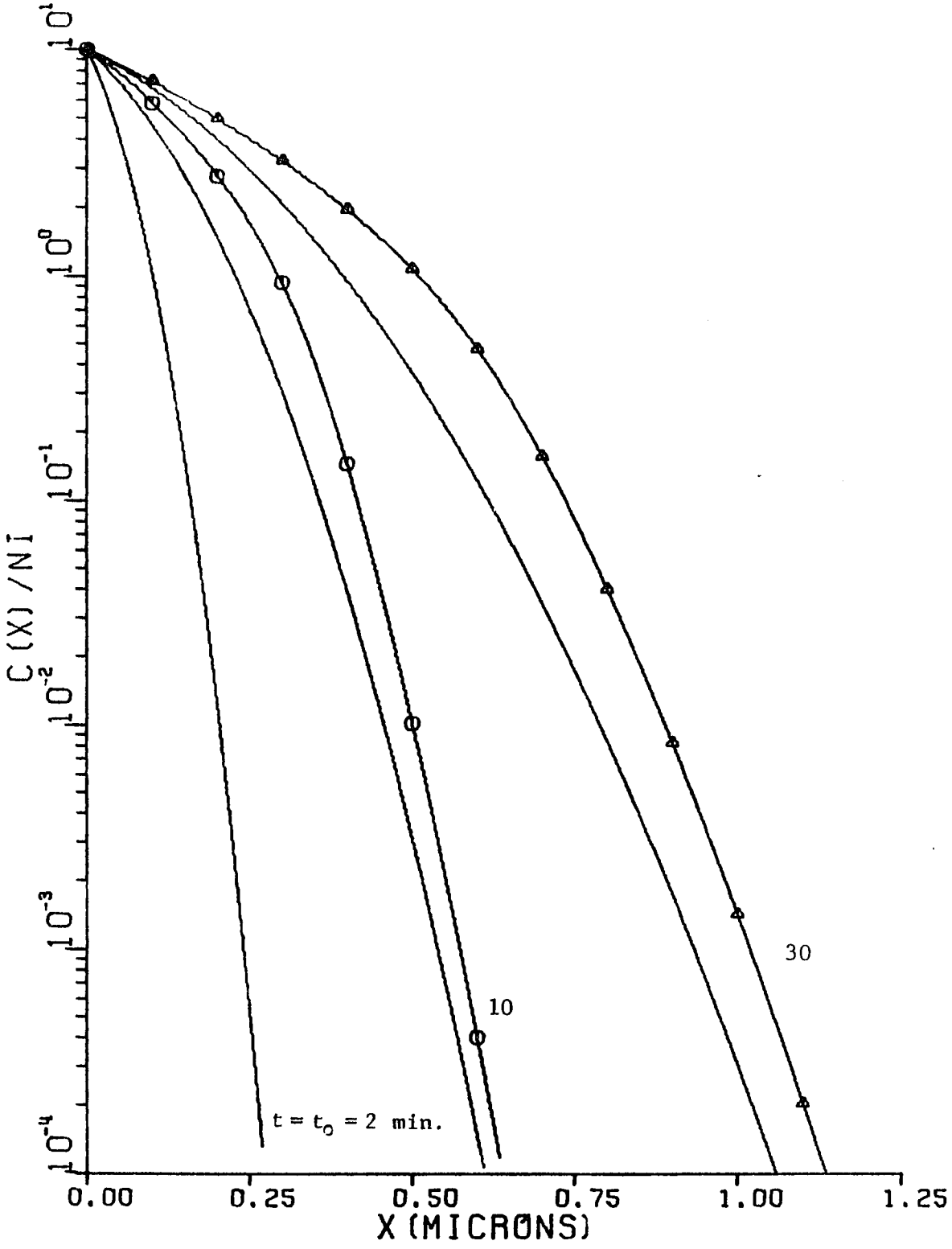

FIGURE 3.3. Impurity profiles for $\beta = 10$; unmarked curves represent profiles when the field is zero.

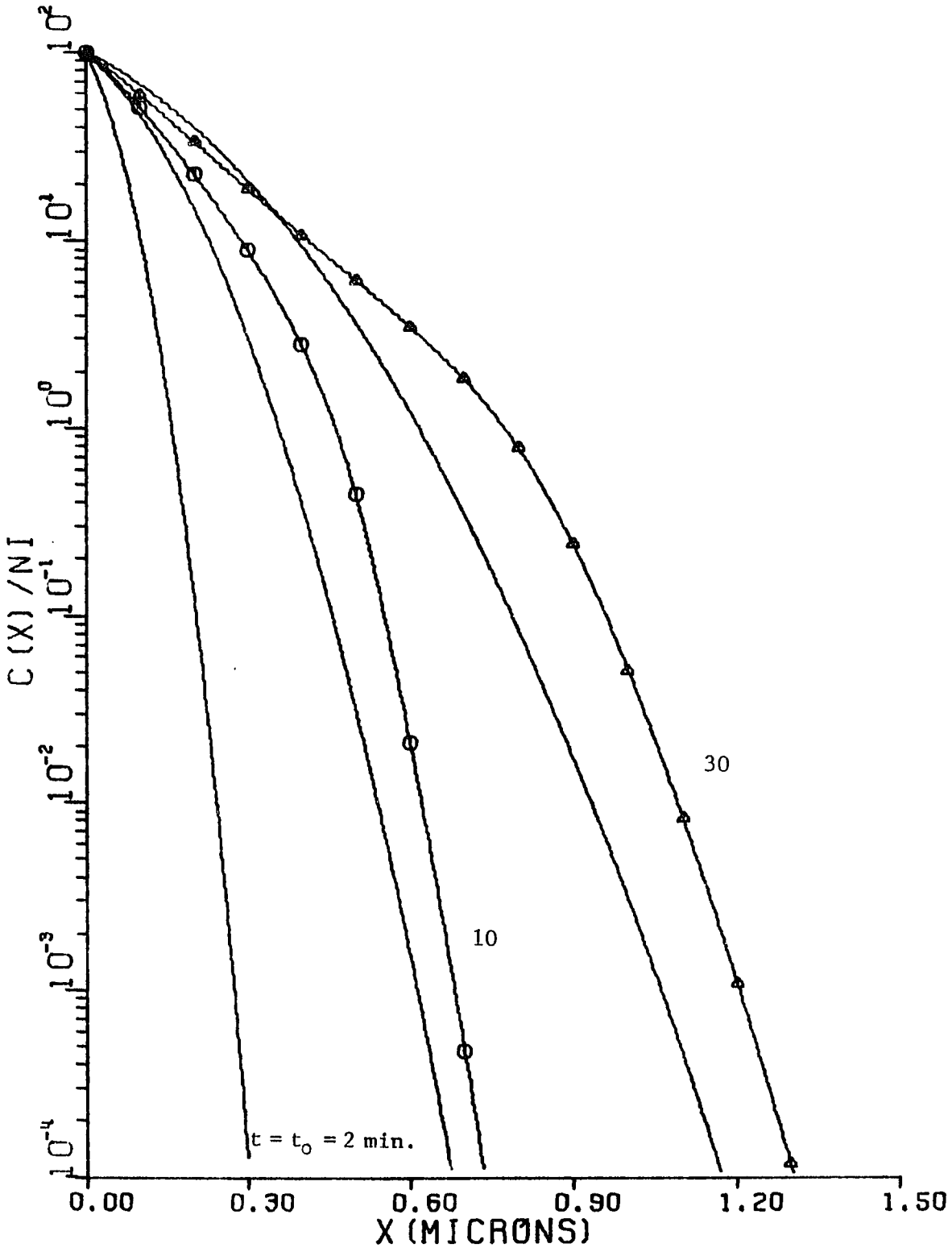

FIGURE 3.4. Impurity profiles for β = 100; unmarked curves represent profiles when the field is zero.

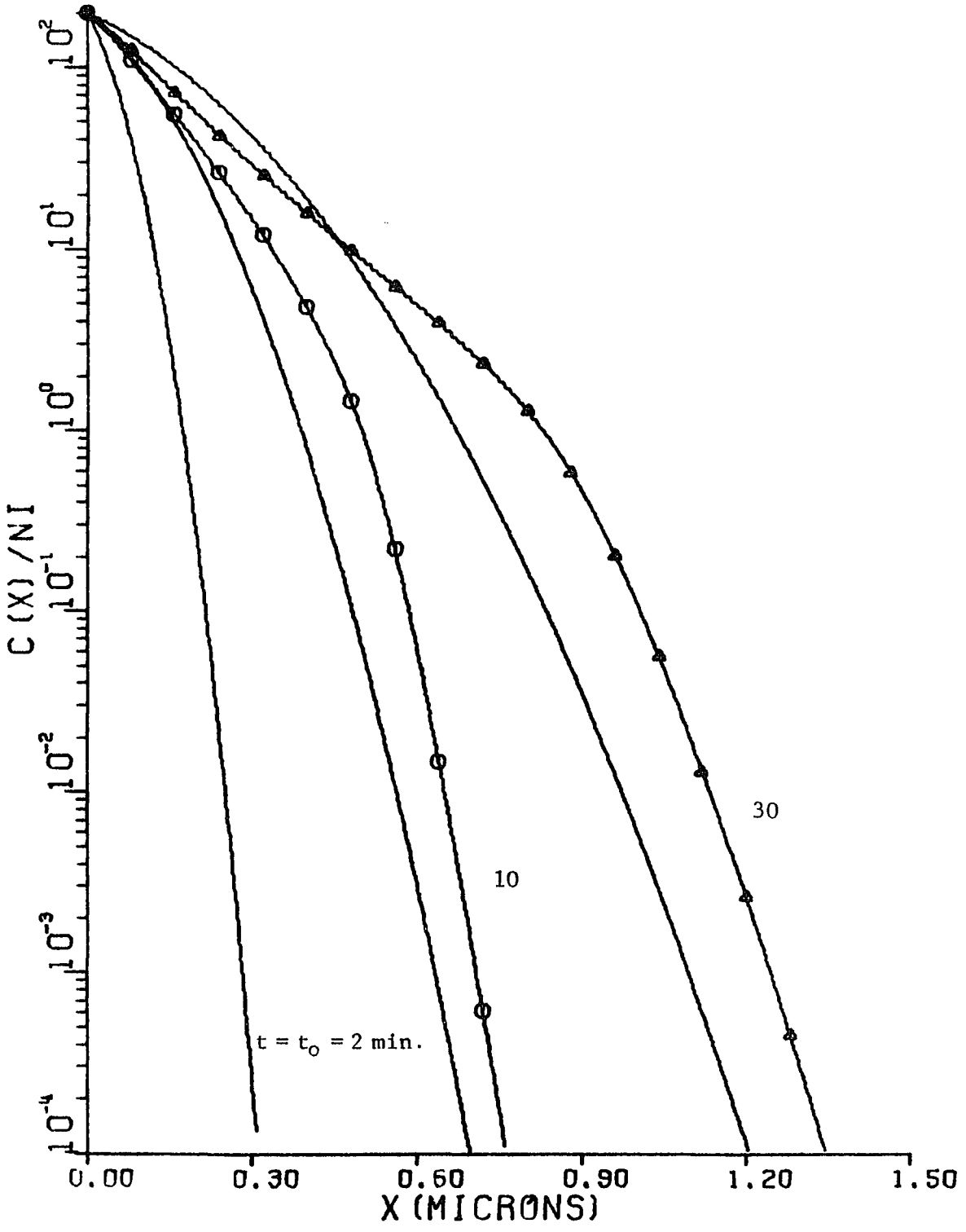

FIGURE 3.5. Impurity profiles for β = 200; unmarked curves represent profiles when the field is zero.

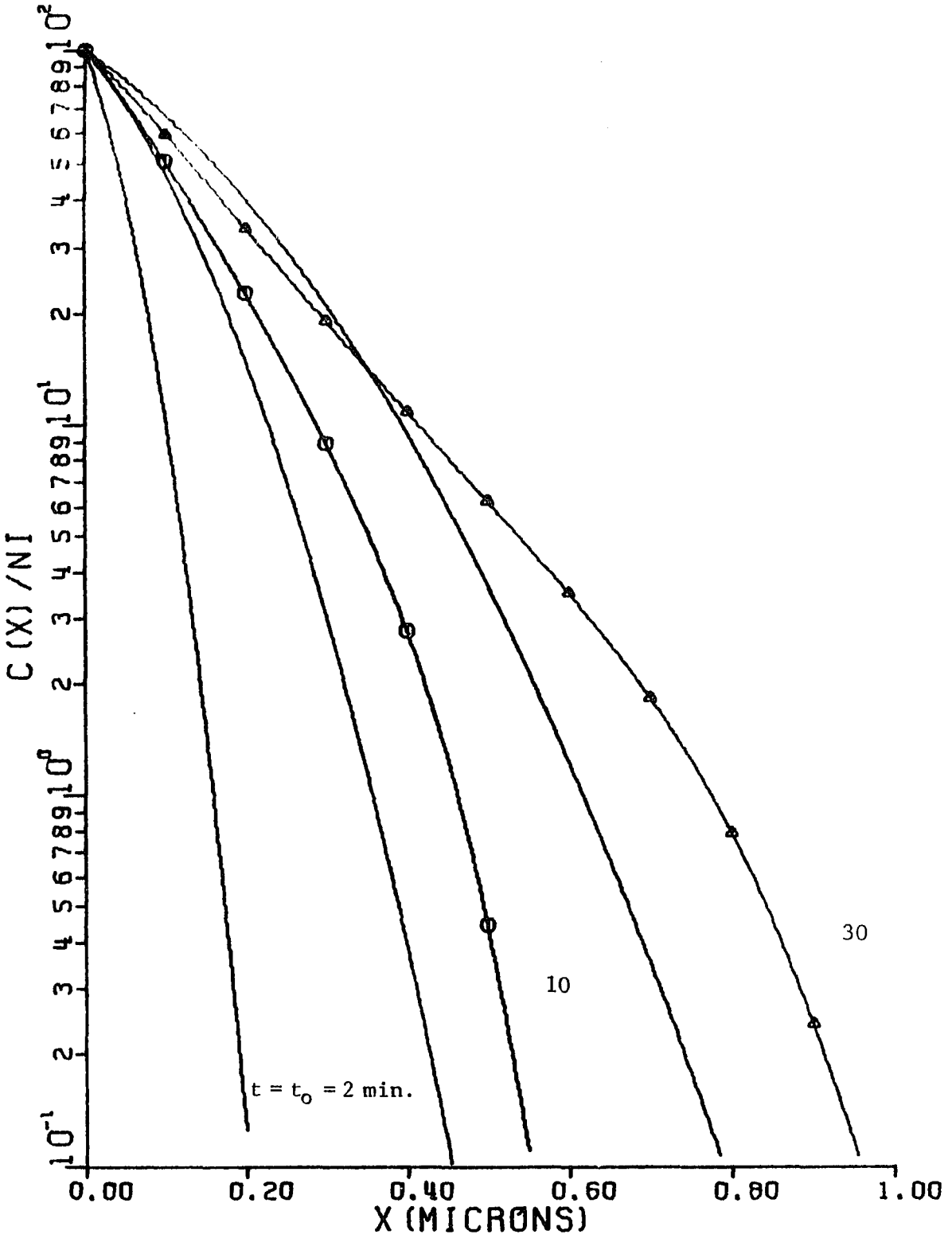

FIGURE 3.6. Expanded view of impurity profiles for β = 100; unmarked curves represent profiles when the field is zero.

In Chapter 1 it was shown that the assumptions of charge neutrality and $pn = n_i^2$ could be used to derive an approximate diffusion equation given by (1-22). When $\beta = 1$, the maximum value of $pn = 1.04n_i^2$. However for $\beta = 10$, the maximum deviation from n_i^2 was approximately 12%. For $\beta = 100$ and 200, the maximum deviation was approximately 18%. In the latter two cases, the maximum value of pn occurred when $c(x,t) \simeq n_i$.

The approximate diffusion equation (1-22) was solved subject to the same boundary conditions and initial values using the iteration method described in Chapter 2. The results are presented in Figures 3.7 through 3.9. Inspection of Figure 3.7 indicates that for $\beta \leq 1$, the approximate diffusion equation yields very good results. This is because the assumptions of charge neutrality and $pn = n_i^2$ are approximately true for $\beta \leq 1$. For the case of $\beta = 10$, (1-22) yields a distribution at $t = 30$ minutes which is somewhat larger than that obtained by solving the transport equations. For $\beta = 100$, the difference between the two solutions is much more pronounced. Note that (1-22) overestimates the actual solution for $\beta > 1$, and that the error increases with time.

The values of the electric field at $t = 30$ minutes obtained from the solution of (1-22) were comparable to those found by solving the transport equations. Over the range $10^2 < E < 10^4$ v/cm, the values from the two solutions at any x differed at most by a factor of 3 or 4 and typically by less than 30%

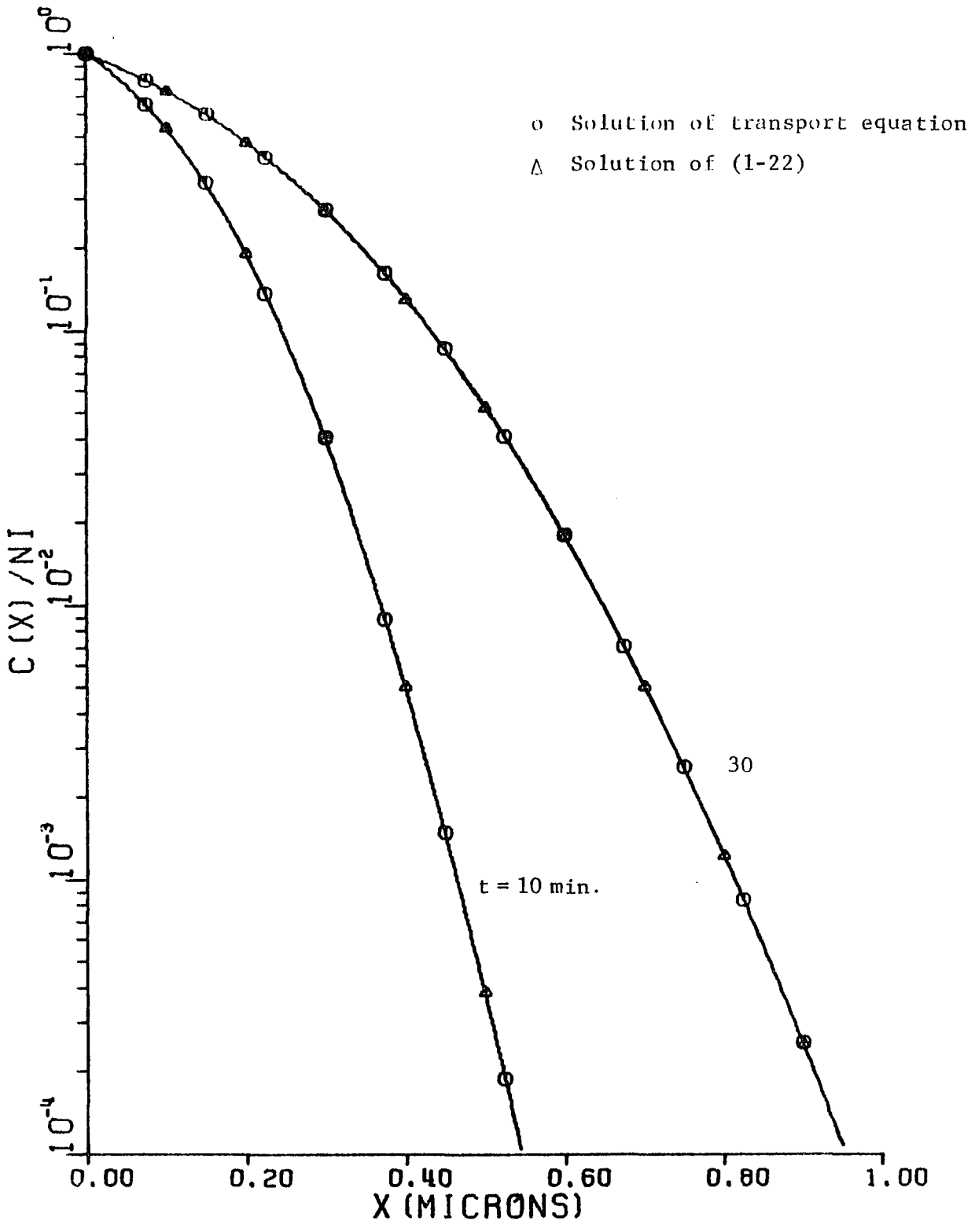

FIGURE 3.7. Impurity profiles obtained by solving the transport equations and the approximate diffusion equation (1-22) for $\beta = 1$.

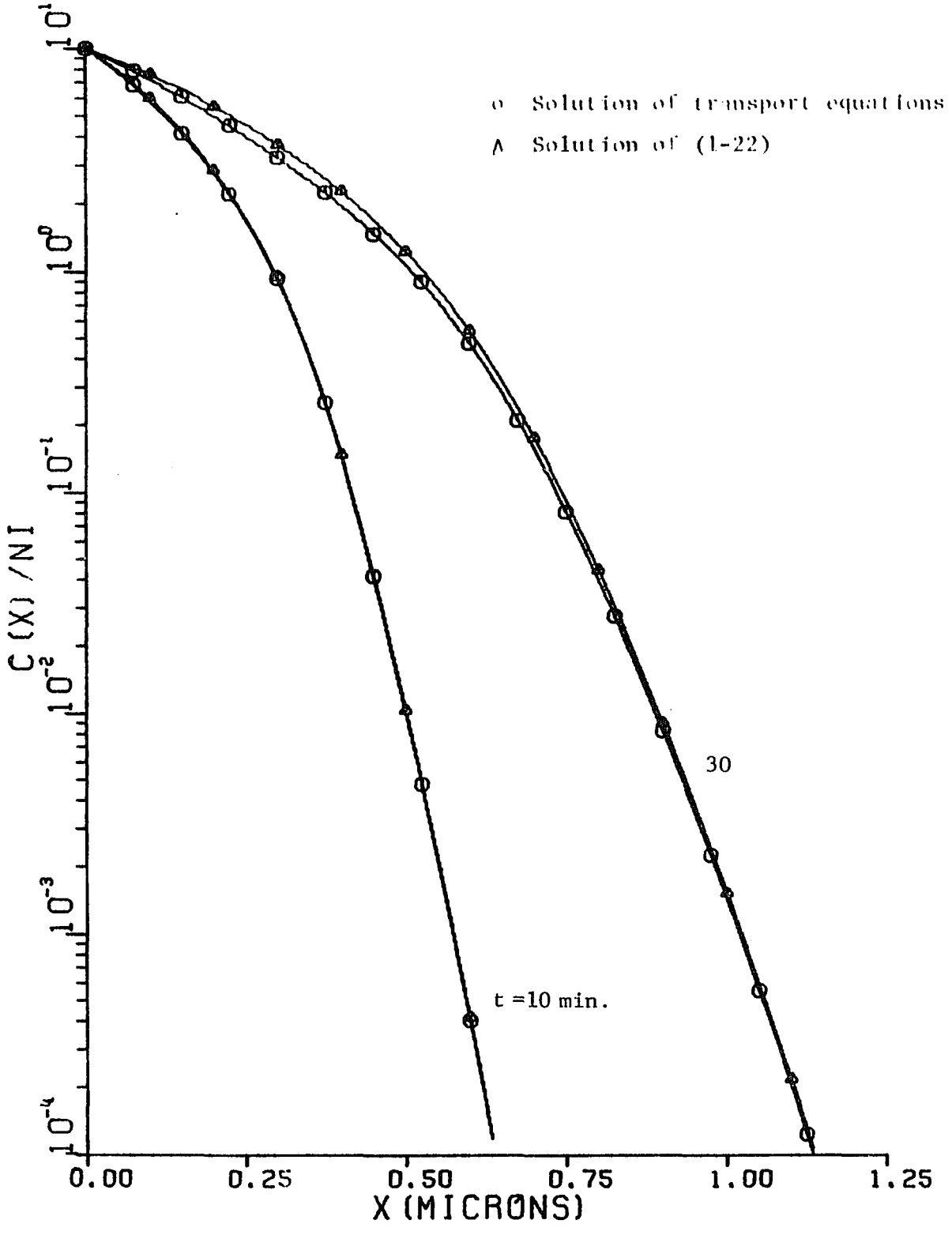

FIGURE 3.8. Impurity profiles obtained by solving the transport equations and the approximate diffusion equation (1-22) for $\beta = 10$.

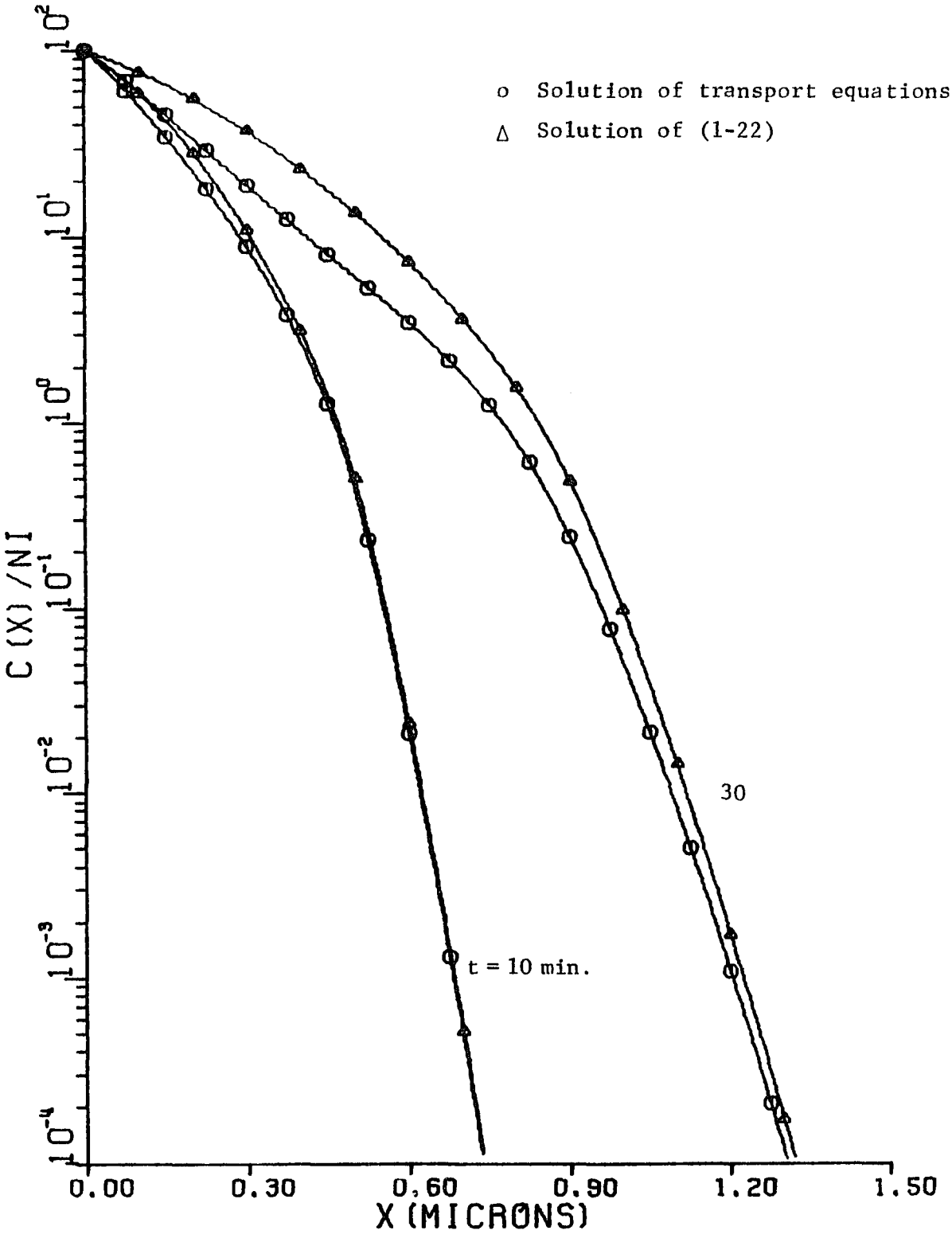

FIGURE 3.9. Impurity profiles obtained by solving the transport equations and the approximate diffusion equation (1-22) for $\beta = 100$.

In Chapter 4 several conclusions are presented based on the results of this study. The problem of degeneracy is briefly discussed and recommendations for further study are made.

Chapter 4

CONCLUSIONS

The objective of this research was to ascertain the behavior of singly ionized impurity atoms diffusing into an initially intrinsic semiconductor. The equations defining the transport model were presented and the appropriate boundary conditions and initial values were discussed. Since these nonlinear equations can not be solved analytically, an iteration scheme was described which can be used to numerically solve the system of equations. Solutions were presented for the case of boron diffusing in silicon at 1100°C. The impurity atoms were assumed to be 100% ionized and the surface concentration C_0 was maintained constant.

The results show that for $C_0/n_i \leq 0.1$ the impurity profile is essentially given by the complementary error function. Note that n_i is a function of temperature and that at 1100°C, $n_i \simeq 10^{19}\,cm^{-3}$. Thus it is concluded that the electric field which arises during the diffusion process has a negligible effect on the motion of the impurity ions for such low values of C_0. However for higher surface concentrations, the internal electric field does have an effect on the diffusion process. The electric field acts to enhance the diffusion of impurity ions in the semiconductor material. For values of C_0/n_i on the order of 100, the impurity profile near the surface was found to be exponentially decreasing with x for diffusion times on the order

of 30 minutes. The range of x for which this is true depends upon the parameters which describe the diffusion process; for example, temperature and surface concentration.

The solutions to the approximate diffusion equation (1-22) were compared to the corresponding solutions obtained from the transport equations. It was found that the approximate diffusion equation is adequate to determine the impurity distribution for values of $C_o/n_i \leq 10$. Adequate in this sense means errors $\leq 25\%$ for diffusion times ≤ 30 minutes. For higher surface concentrations, the results obtained using (1-22) show considerable deviation from those obtained by solving the system of nonlinear equations. For example, for $C_o/n_i = 100$, errors of over 100% were found for some values of x at $t = 30$ minutes. The deviation between the two solutions increased as C_o was increased. One possible explanation for this effect is that the assumption $pn = n_i^2$, which was used in the derivation of (1-22), becomes less valid as C_o increases.

For $C_o/n_i \leq 0.1$ the numerical solution reduces to the known correct solution, thus giving confidence in the accuracy of the numerical technique. As another check on the accuracy of the numerical scheme, the net charge was computed using the calculated distirubutions of holes, electrons and impurity ions. Since no net charge is added to the semiconductor, during the diffusion process, the material must be charge neutral. The semiconductor material as a whole was found to be charge neutral within the accuracy of the numerical technique for all values of C_o used.

Thái [10] has pointed out that when the acceptor impurity concentration becomes comparable to N_V, the effective density of states in the valence band, the product $pn > n_i^2$ due to degeneracy. The value of N_V for boron at 1100^oC is approximately $10^{20} cm^{-3}$. Thus the results for $C_O > 10^{20}$ are open to question due to the use of $pn = n_i^2$ in determining the boundary conditions at $x = 0$.

The numerical results presented in Chapter 3 were obtained using the first unified approach to the study of field-aided diffusion. Furthermore, it was also shown that the concept of an "effective" diffusion coefficient discussed in Chapter 1 is meaningful for values of $C_O/n_i \leq 10$. The numerical approach described in Chapter 2 is applicable to a wide variety of problems similar to the one studied here.

There are several areas in which this basic numerical technique can be applied. Most semiconductor devices are fabricated using two diffusion steps. The second diffusion takes place in a semiconductor which already contains impurity ions and a built in electric field. The impurity ions used in the second diffusion are usually of the opposite type to those used in the first diffusion step. Therefore a pn junction will be formed whose location is a function of the diffusion time. It is not known to what extent the internal electric field generated during the second diffusion will effect the original impurity profile and therefore, the location of the junction.

Another problem of interest would be to use the analysis of Thái to determine a better value of pn suitable for degenerate material and determine the impurity distributions using the new

boundary values at $x = 0$. Note that the basic numerical technique would not change; the use of more accurate boundary conditions at $x = 0$ will yield a more accurate solution. When dealing with degenerate material, the transport model must be re-examined. For example, it is not clear whether the particle flux can even be divided into drift and diffusion terms. The concept of total ionization of the impurity atoms must also be re-examined and a new Einstein relation must be used to relate the mobility and diffusion coefficients [16].

Basic research such as that presented here and recommended above will lead to a better understanding of the basic diffusion process which is so widely used today. This increased understanding may lead to improvement in device performance through optimization of device parameters.

Appendix A

BOUNDARY CONDITIONS AT THE SURFACE

The generalized boundary conditions for holes, electrons, and impurity ions at $x = 0$ are given by

$$c(0,t) = C_o \tag{A-1}$$

$$p(0,t) = f(t) \tag{A-2}$$

$$n(0,t) = g(t) \tag{A-3}$$

where C_o is the constant surface concentration of impurity ions, assumed constant, and f(t) and g(t) are appropriate functions of time. Let us consider at time $t = 0$ that C_o impurity ions per cm^3 exist at $x = 0$ and that no diffusion or recombination has taken place. If the ions are acceptor type impurity ions, then

$$f(0) = n_i + C_o \tag{A-4}$$

and

$$g(0) = n_i \tag{A-5}$$

where n_i is the intrinsic concentration of holes and electrons. Now as t increases, the impurity ions and holes diffuse away from the surface. Recombination will also take place; thus f(t) and g(t) will both decrease from their values at $t = 0$.

There is no known way to determine f(t) and g(t). An attempt was made to use the continuity equations for p and n; however, these

equations could not be successfully used to determine the boundary conditions. The continuity equations for holes and electrons are given by

$$\frac{\partial p}{\partial t} = D_p\left[\frac{\partial^2 p}{\partial x^2} - \frac{1}{V_T}\frac{\partial}{\partial x}(pE)\right] + G \qquad \text{(A-6)}$$

and

$$\frac{\partial n}{\partial t} = D_n\left[\frac{\partial^2 n}{\partial x^2} + \frac{1}{V_T}\frac{\partial}{\partial x}(nE)\right] + G \qquad \text{(A-7)}$$

Let $r(x,t)$ represent the right hand side of (A-6). Using a forward difference formula for $\frac{\partial p}{\partial t}$ at $t=0$ yields

$$\frac{p(0,t_1) - p(0,0)}{\Delta t} \simeq \left.\frac{\partial p(0,t)}{\partial t}\right|_{t=0} = r(0,0)$$

so that $p(0,t_1)$ is found easily as

$$p(0,t_1) = p(0,0) + \Delta t\, r(0,0) \qquad \text{(A-9)}$$

and in general

$$p(0,t_k) = p(0,t_k-\Delta t) + \Delta t\, r(0,t_k-\Delta t) \qquad \text{(A-10)}$$

A similar expression was derived for $n(0,t_k)$ using (A-7).

It was found that this technique yields values of $p(0,t)$ which increase monotonically with time. The problem stems from the fact that a one sided formula must be used to compute $\frac{\partial^2 p}{\partial x^2}$. When this is done, $\frac{\partial^2 p}{\partial x^2} > 0$ and is the dominant term. Thus $p(0,t)$ is larger after the first time step which leads to a larger $r(0,t)$ which yields an

even larger value of $p(0,t)$ at the next instant of time. No implicit scheme such as that employed to determine $p(x,t)$, $n(x,t)$ and $c(x,t)$ for $0 < x < L$ was found to determine the boundary values.

Since the concentration of impurity ions at $x = 0$ is assumed constant and the lifetimes of holes and electrons are on the order of nanoseconds, it is reasonable to expect that within a very short time, a steady-state condition will be established at the surface. If we assume that $f(t)$ and $g(t)$ have reached their steady-state values after approximately one second of diffusion time, then the boundary values will be constant throughout the remainder of the diffusion process.

In order to find these steady-state values, consider the following two equations

$$p(0,t) - n(0,t) + zC_o = \rho_o/e$$

$$p(0,t)\, n(0,t) = bn_i^2$$

where ρ_o is the net charge density at $x = 0$, b is a measure of the deviation of the product $p(0,t)\, n(0,t)$ from its thermal equilibrium value, and $z = -1$ for acceptor impurities and $+1$ for donor impurities. When thermal equilibrium conditions exist at $x = 0$, $b = 1$.

Solving the above two equations simulatneously for $p(0,t)$ and $n(0,t)$ yields

$$p(0,t) = -\frac{1}{2} U + \frac{1}{2}\left[U^2 + 4bn_i^2\right]^{1/2} \qquad \text{(A-8)}$$

$$n(0,t) = \frac{1}{2} U + \frac{1}{2}\left[U^2 + 4bn_i^2\right]^{1/2} \qquad \text{(A-9)}$$

where $$U = zC_o - \rho_o/e = (zeC_o - \rho_o)/e \qquad \text{(A-10)}$$

Now zeC_o is the charge density due to the impurity ions while ρ_o is the net charge density. It is reasonable to expect that the net charge density would be much less than that due to the impurity atoms alone. Any deviation from charge neutrality would be accompanied by an electric field. This electric field would tend to cause the mobile holes and electrons to move in such a way as to restore change neutrality. Thus the following assumption seems justified:

$$|zeC_o| \gg |\rho_o| \qquad \text{(A-11)}$$

therefore $$U = zC_o \qquad \text{(A-12)}$$

There is no known way to determine the exact value of b. The semiconductor material is certainly not in thermal equilibrium during the diffusion process; however, there has been no evidence published to date which would lead to the conclusion that b is significantly different from unity unless the material becomes degenerate. Therefore the only way to determine the effect of b on the impurity distribution at any time t is by a sensitivity analysis. The transport equations were solved as described in Chapter 2 with $C_o = 10^{20}\ cm^{-3}$ for the case of boron atoms as discussed in Chapter 3. Values of b = 0.5, 1 and 2 were used. The impurity profiles after 30 minutes of diffusion time were compared and it was found that the profiles for b = 0.5 and 2 differed by approximately 5% from that obtained for b = 1. Although this sensitivity analysis was not extensive a value

of $b = 1$ was chosen for all cases described in Chapter 3. By using (A-12) and $b = 1$ in (A-8) and (A-9), the boundary conditions given by (2-7) follow immediately.

Appendix B

INITIAL CONDITIONS

The initial conditions at time $t = 0$ prior to the diffusion of the impurity ions are given by

$$p(x,0) = n_i, \quad 0 < x < L \tag{B-1}$$

$$n(x,0) = n_i \tag{B-2}$$

$$c(x,0) = 0 \tag{B-3}$$

and

$$E(x,0) = 0, \quad 0 \leq x \leq L \tag{B-4}$$

Numerical difficulties were encountered when these initial conditions were used. The difficulty stems from the very large changes which occur in the impurity ion concentration near the surface early in the diffusion process. As described in Chapter 2, the x and t coordinates are divided into discrete points. Consider $c(x_2,t_1)$ where $x_2 = x_1 + \Delta x$, $x_1 = 0$, $t_1 = t_o + \Delta t$ and $t_o = 0$. Thus $c(x_2,t_1)$ represents the value of the impurity ion centration a distance Δx from the surface at the end of the first time step. With a Δt of 0.5 seconds, and Δx on the order of 0.005 microns, the program calculates a value of $c(x_2,t_1)$ which is almost equal to $c(x_1,t_1) = C_o$. Now C_o is on the order of 10^{19} cm^{-3} so that in 0.5 seconds, the impurity ion concentration at $x = \Delta x$ goes from 0 to almost 10^{19} cm^{-3}. The changes which occur in c

for $x > \Delta x$ decrease with increasing x. As described in Chapter 2, the numerical scheme uses a finite difference approximation for $\partial c/\partial t$ in the calculation of $c(x,t_1)$. For any value of x,

$$\left.\frac{\partial c(x,t)}{\partial t}\right|_{t_1} = \frac{c(x,t_1) - c(x,t_0)}{\Delta t}$$

When such large changes occur in c, this approximation becomes quite poor so that errors are introduced in the calculation of $c(x,t_1)$. Furthermore since $c(x,t_1)$ becomes the starting condition in the calculation of $c(x,t_2)$, the values of $c(x,t_2)$ will also be incorrect. The hole and electron distributions will also be in error due to the coupled nature of the transport equations.

This numerical difficulty is avoided if the program is started at some time greater than $t = 0$ such that the large changes in the impurity concentration discussed above do not occur. We must, therefore, choose hole, electron, impurity ion and electric field distributions at some starting time t_s. Due to the iterative nature of the numerical technique used to solve the transport equations, these distributions need not be exact distributions at time t_s. The following starting conditions were selected:

$$c(x,t_s) = C_o \text{ erfc } \left[x(4D_c t_s)^{-1/2}\right] = \varphi(x) \qquad \text{(B-5)}$$

$$p(x,t_s) = -\frac{z}{2}\varphi + (\varphi^2 + 4n_i^2)^{1/2} \qquad \text{(B-6)}$$

$$n(x,t_s) = \frac{z}{2}\varphi + (\varphi^2 + 4n_i^2)^{1/2} \qquad \text{(B-7)}$$

$$E(x,t_s) = -z V_T \frac{1}{\varphi}\left[1 + \left(\frac{2n_i}{\varphi}\right)^2\right]^{-1/2} \frac{\partial\varphi}{\partial x} \qquad \text{(B-8)}$$

where $t_s = 120$ seconds.

In order to obtain the above equations, several assumptions were made. The first assumption is that the internal electric field has not had time to cause a significant deviation in the particle distributions after only 120 seconds of diffusion time; thus $c(x,t_s)$ is given by the complementary error function. The second assumption is that the net charge density at any point is much less than the charge density due to the impurity ions alone. The net charge density $\rho(x,t_s)$ is given by

$$p(x,t_s) - n(x,t_s) + zc(x,t_s) = \frac{\rho(x,t_s)}{e}$$

By our second assumption,

$$p(x,t_s) - n(x,t_s) = \frac{\rho(x,t_s) - zec(x,t_s)}{e} \simeq -zc(x,t_s) \qquad \text{(B-9)}$$

By arguments similar to those given in Appendix A, it is reasonable to assume that

$$p(x,t_s)\, n(x,t_s) = n_i^2 \qquad \text{(B-10)}$$

Using (B-9) and (B-10), (B-6) and (B-7) follow immediately. Equation (B-8) was derived in section (1-2). It should be noted that these are not the only starting conditions which could be used. These are only used to start the iteration process. It was found the using $E(x,t_s) = 0$

yielded the same particle distributions at $t = 3$ minutes as using (B-8).

In order to determine whether this set of starting conditions was actually appropriate to use, impurity profiles were obtained using (B-5) - (B-8) with $C_o = 10n_i$ and $t_s = 10$ seconds. These profiles were different from those obtained using $t_s = 120$ seconds for $t < 3$ minutes; however, the differences decreased with time and at $t = 30$ minutes, the profiles were almost identical. This indicated that a $t_s = 120$ seconds was adequate to determine $c(x,t)$ for $t > 3$ minutes. Using the larger value of t_s resulted in a considerable savings in computer time.

Appendix C

PROGRAM INFORMATION

The computer program used to obtain the results reported in Chapter 3 is given below. The program is written in the FORTRAN-IV programming language and was implemented on a IBM S/360 computer. Input data requirements and program control options are described in C.1; a source program listing is given in C.2.

C.1. User's Guide

The user must provide values for the following parameters found in the program under the heading "INPUT DATA." All values should be entered using the format shown in the program listing.

TO	Starting time in seconds
BETA	$c(0,t)/n_i$
TEMP	Diffusion temperature in degrees centigrade.
NSUBI	n_i, the intrinisc concentration of free electrons at the diffusion temperature per cm^3.
GAMMA	Parameter defined by $p(0,t)n(0,t) = \gamma n_i^2$.
DSUBP	Diffusion constant for holes, D_p, in cm^2/sec.
DSUBN	Diffusion constant for electrons, D_n, in cm^2/sec.
TAUP	Lifetime for holes, τ_p, in seconds.
TAUN	Lifetime for electrons, τ_n, in seconds.

DSUBC — Diffusion constant for impurity ions, D_c, in cm^2/sec.

Z — +1 for a donor type impurity
-1 for an acceptor type impurity

In addition to the above information, the user must also provide values for the following parameters listed in the program under the heading "PROGRAM CONTROL."

DX1 — Δx in microns.

APROXL — Approximate value for L in microns. The exact value is determined by the program as $m\Delta x$, where m is a integer such that $m\Delta x \geq$ APROXL

DT1 — Δt in seconds.

TSTOP — Maximum diffusion time in seconds.

CKC — Parameter used in the accuracy check. Distributions are assumed accurate enough when $\Delta\delta^{j+1}(x_i, t_k) / \delta^j(x_i, t_k) \leq$ CKC for all i, where δ represents p, n or c.

CNORM — Normalization factor for particle concentrations, n_1. The program uses $n_1 = 10^{10} cm^{-3}$.

CSTOP — Minimum value of c(x,t) allowed. Smaller values are set equal to zero to avoid underflow errors. The program uses CSTOP = $10^{-10} cm^{-3}$.

ESTOP — Minimum value of E(x,t) allowed. Smaller values are set equal to zero to avoid underflow errors. The program uses ESTOP = 10^{-10} V/cm.

DTPRNT — Values of p, n, c, E, charge density, and current density components are all printed out when time t is an integral multiple of DTPRNT seconds.

DTPUN — Values of c(x,t) are punched out on cards when t is an integral multiple of DTPUN seconds.

The values of $p(x_i, t_k)$ are stored in an array. The maximum number of elements in this array is set by a dimension statement as 502. All other dimensioned variables are also limited to 502 elements each.

C.2. Program Listing

```
C    PROGRAM FOR THE STUDY OF FIELD-AIDED DIFFUSION
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 N,NO,NI,NSUBI,JNORM,NSUBIN,NISQN
      REAL*8 JPDRI,JPDIF,JNDRI,JNDIF,JN,JP,JCDRI,JCDIF,JC
      DIMENSION P(502),N(502),C(502),E(502)
      DIMENSION PO(502),NO(502),CO(502),EO(502)
      DIMENSION DP(502),DDP(502),DN(502),DDN(502),DC(502),DDC(502)
      DIMENSION G(502),H(502),DLTA(502),X(502)
C
C ***************************************************************
C
C *************** INPUT DATA ********************************
C
      TO=120.D0
      BETA=1.D0
      TEMP=1100.D0
      NSUBI=1.D19
      GAMMA=1.D0
      DSUBP=2.0D0
      DSUBN=6.0D0
      TAUP=1.D-9
      TAUN=1.D-9
      DSUBC=1.6D-13
      Z=-1.D0
C
C   BETA = C(0+,T)/NSUBI
C
C ***************************************************************
C
C ***** PROGRAM CONTROL ***************************
C
      DX1=0.005D0
      APROXL=2.D0
      DT1=0.5D0
```

```
      TSTOP=30.01D0*60.D0
      CKC=1.D-4
      CNORM=1.D10
      CSTOP=1.D-10
      ESTOP=1.D-10
      DTPRNT=10.D0
      DTPUN=300.D0
C
C     DISTRIBUTIONS ARE PRINTED OUT WHEN TIME T IS AN INTEGRAL MULTIPLE
C        OF 'DTPRNT' SECONDS
C     DISTRIBUTIONS ARE PUNCHED OUT WHEN TIME T IS AN INTEGRAL MULTIPLE
C        OF 'DTPUN' SECONDS
C
C ***********************************************************************
C
C **** NORMALIZATION CONSTANTS FOR SILICON *******
C
      BK=1.381D-23
      ECHRGE=1.602D-19
      EPSLON=1.0000D-12
      DNORM=1.D0
      VSUBT=BK*(TEMP+273.D0)/ECHRGE
      XNORM=DSQRT(EPSLON*VSUBT/(ECHRGE*CNORM))
      TNORM=XNORM*XNORM/DNORM
      ENORM=VSUBT/XNORM
      VNORM=VSUBT
      JNORM=ECHRGE*CNORM*DNORM/XNORM
      QNORM=ECHRGE*CNORM
      XNORMM=XNORM*1.D4
C
C ***** OTHER CONSTANTS USED IN CALCULATIONS *****
C
      DX2=2.D0*DX1
      CXEO=BETA*NSUBI
      CSTOPN=CSTOP/CNORM
      NSUBIN=NSUBI/CNORM
```

```
      NISQN=NSUBIN*NSUBIN
      CONST=4.D0*NISQN
      DLTSTP=CSTOPN
      ESTOPN=ESTOP/ENORM
      OODP=1.D0/DSUBP
      OODN=1.D0/DSUBN
      OODC=1.DC/DSUBC
      TP=TAUP/TNORM
      TN=TAUN/TNORM
      DX=DX1/XNORMM
      IDTPRN=DTPRNT*100.D0+0.1D0
      IDTPUN=DTPUN*100.D0+0.1D0
C
C ***************************************************************************
C
C ***** CALC. OF X(I), NO. STEPS AND EXACT LENGTH **********
C
      X(1)=0.D0
      DO 10 I=2,1000
      J=I-1
      X(I)=X(J)+DX1
      IF(X(I).GT.APROXL) GO TO 11
   10 CONTINUE
   11 XL=X(J+1)
      NS=J
      NP=NS+1
      NPM1=NP-1
      NPM2=NP-2
      N100=(NP+60)/100
      N101=N100+1
C
C ***************************************************************************
C
C *********** PRINTOUT OF TITLE PAGE *************
C
      PRINT 600
```

```
      IF(Z.LT.0.D0) GO TO 2
      PRINT 608
      GO TO 3
    2 PRINT 609
    3 CONTINUE
      PRINT 615,BETA
      PRINT 601,XL
      PRINT 602,DX1
      PRINT 603,NP
      PRINT 604,TEMP
      PRINT 605,NSUBI
      PRINT 606,DSUBP
      PRINT 607,DSUBN
      PRINT 612,TAUP,TAUN
      PRINT 610,DSUBC
      PRINT 611,CXE0
      CKCPC=CKC*100.D0
      PRINT 613,CKCPC
      PRINT 614
      PRINT 213
C
  600 FORMAT(//5X,'TRANSIENT ANALYSIS PROGRAM FOR FIELD-AIDED DIFFUSION'
     1,////)
  601 FORMAT(5X,'LENGTH = ',F8.4,' MICRONS'/)
  602 FORMAT(5X,'DELTA X = ',F8.4,' MICRONS'/)
  603 FORMAT(5X,'TOTAL NUMBER OF POINTS = ',I4////)
  604 FORMAT(5X,'TEMPERATURE = ',F10.1,' DEGREES CENTIGRADE'/)
  605 FORMAT(5X,'INTRINSIC CONC. OF ELECTRONS = ',1PD10.2,' PER CUBIC CM
     1.'/)
  606 FORMAT(5X,'DIFFUSION CONSTANT FOR HOLES = ',1PD10.2/)
  607 FORMAT(5X,'DIFFUSION CONSTANT FOR ELECTRONS = ',1PD10.2///)
  608 FORMAT(5X,'DIFFUSION OF DONOR IMPURITY IONS IN SILICON'//)
  609 FORMAT(5X,'DIFFUSION OF ACCEPTOR IMPURITY IONS IN SILICON'//)
  610 FORMAT(5X,'DIFFUSION CONSTANT FOR IMPURITY IONS = ',1PD13.3/)
  611 FORMAT(5X,'SURFACE CONCENTRATION, C(0,T) = ',1PD10.2////)
  612 FORMAT(5X,'LIFETIMES,  TP = ',1PD10.2,' SEC.',6X,'TN = ',1PD10.2,
```

```
     1   ' SEC.'///)
  613 FORMAT(5X,'CONVERGENCE CHECK--IF ON ANY ITERATION P, N AND C CHANG
     1E BY LESS THAN ',F5.3,' PERCENT'/, 24X,'PROGRAM PROCEEDS TO THE NE
     1XT TIME STEP'//////)
  614 FORMAT(5X,'DECK  DIFF1C')
  615 FORMAT(5X,'BETA = ',F7.2//)
C
      T=TO
      K=0
      ITER=0
      DELTAT=DT1
C
C ***************************************************************************
C
C     BOUNDARY CONDITIONS FOR C(X),P(X) AND N(X) FOR ALL TIME
C
C     VALUES AT X = 0
C     MODEL--P(X)*N(X)=NSUBI*NSUBI AND RHO = 0
C
      CO(1)=CXEO/CNORM
      PO(1)=(-Z*CO(1)+DSQRT(CO(1)*CO(1)+4.D0*NISQN*GAMMA))/2.D0
      NO(1)=NISQN*GAMMA/PO(1)
C
C     VALUES AT X = L
C     MODEL -- THERMAL EQUILIBRIUM AND INTRINSIC MATERIAL
C
      CO(NP)=0.D0
      PO(NP)=NSUBIN
      NO(NP)=NSUBIN
C
C ***************************************************************************
C
C     STARTING CONDITIONS FOR C(X),E(X),P(X) AND N(X)
C     MODEL -- RHO IS CONSTANT, P(X)*N(X)=NSUBI*NSUBI, AND
C              C(X) MUCH MUCH GREATER THAN RHO/(1.6E-19 COUL.)
C
```

```
C       IMPURITY ATOM DISTRIBUTION CO(X)
C       COMPLEMENTARY ERROR FUNCTION ASSUMED
C
        C1=CXEO/CNORM
        XX=DSQRT(4.D0*DSUBC*T)*1.D4
        DO 4 I=2,NPM1
        CO(I)=C1*DERFC(X(I)/XX)
        IF(CO(I).LT.CSTOPN) GO TO 5
    4   ISTOP=I
    5   ISTOP1=ISTOP+1
        DO 6 I=ISTOP1,NPM1
    6   CO(I)=0.D0
C
C       ELECTRIC FIELD DISTRIBUTION EO(X)
C
        CALL DERIV(CO,G,DX,NP)
        DO 7 I=1,NP
    7   EO(I)=-Z*G(I)/DSQRT(CO(I)*CO(I)+CONST)
C
C       CALCULATION OF NORMALIZED CHARGE DENSITY G(X) FROM EO(X)
C
        CALL DERIV(EO,G,DX,NP)
C
C       ELECTRON AND HOLE DISTRIBUTIONS NO(X) AND PO(X)
C
        DO 9 I=2,ISTOP
        PO(I)=(-Z*CO(I)+DSQRT(CO(I)*CO(I)+4.D0*NISQN))/2.D0
        NO(I)=NISQN/PO(I)
    9   CONTINUE
        DO 14 I=ISTOP1,NPM1
        PO(I)=NSUBIN
   14   NO(I)=NSUBIN
C
C ***************************************************************************
C
   16   LASTI=ISTOP+10
```

```
      IF(LASTI.GT.NP) LASTI=NP
      LSTIM1=LASTI-1
C
C     INITIALIZE E(X) ARRAY
C
      DO 15 I=1,NP
   15 E(I)=0.D0
C
C ***************************************************************************
C
C ***** PRINT OUT OF STARTING DISTRIBUTIONS ****************
C
      Y=T/60.D0
      PRINT 650,T,Y
      PRINT 652,K
      PRINT 653,ITER
      PRINT 651
      DO 20 I=1,N100
      A1=P0(I)*CNORM
      A2=N0(I)*CNORM
      A3=C0(I)*CNORM
      A4=G(I)*QNORM
      A5=E0(I)*ENORM
   20 PRINT 303,I,X(I),A1,A2,A3,A4,A5
      DO 21 I=N101,NPM1,N100
      A1=P0(I)*CNORM
      A2=N0(I)*CNORM
      A3=C0(I)*CNORM
      A4=G(I)*QNORM
      A5=E0(I)*ENORM
   21 PRINT 303,I,X(I),A1,A2,A3,A4,A5
      A1=P0(NP)*CNORM
      A2=N0(NP)*CNORM
      A3=C0(NP)*CNORM
      A4=G(NP)*QNORM
      A5=E0(NP)*ENORM
```

```
      PRINT 303,NP,X(NP),A1,A2,A3,A4,A5
C
  650 FORMAT(5X,'STARTING DISTRIBUTIONS',5X,'TIME =',F9.2,' SEC, OR'
     1,F10.3,' MIN.'//)
  651 FORMAT(6X,'X(MICRONS)',6X,'P(X)',12X,'N(X)',14X,'C(X)',11X,
     1   ' DD/DX ', 9X,'E-FIELD'//)
  652 FORMAT(6X,'NUMBER OF TIME STEPS THUSFAR, K = ',I6/)
  653 FORMAT(6X,'NUMBER OF ITERATIONS THUSFAR = ',I6//)
C
C ***************************************************************************
C
C ***** ESTIMATED DISTRIBUTIONS AT END OF FIRST TIME STEP *****
C
      DO 12 I=1,NP
      P(I)=PO(I)
      N(I)=NO(I)
   12 C(I)=CO(I)
C
C ***************************************************************************
C
C
   27 K=K+1
C
      T=T+DELTAT
      IF(T.GT.TSTOP) GO TO 999
      IT100=T*100.D0+0.1D0
      DT=DELTAT/TNORM
C
      DTI=1.D0/DT
      OODPDT=DTI*OODP
      OODNDT=DTI*OODN
      OODCDT=DTI*OODC
C
      INDX=0
      J=0
   26 J=J+1
```

```
      ITER=ITER+1
      JFLAG=0
C
      CALL FASDER(P,DP,DDP,DX,LASTI)
      CALL FASDER(N,DN,DDN,DX,LASTI)
      CALL FASDER(C,DC,DDC,DX,LASTI)
C
      DO 28 I=1,LASTI
      E(I)=(EO(I)*DTI-DSUBN*DN(I)+DSUBP*DP(I)+Z*DSUBC*DC(I))/
     1 (DSUBN*N(I)+DSUBP*P(I)+DSUBC*C(I)+DTI)
      IF(DABS(E(I)).LT.ESTOPN) E(I)=0.D0
   28 CONTINUE
      LSTIP1=LASTI+1
      DO 29 I=LSTIP1,NP
   29 E(I)=0.D0
C
C  ***** CALC. OF IMPROVED P(X) ********************
C
      CALL DELTA(1.D0,P,PO,DP,DDP,OODP,OODPDT,P,N,C,E,Z,G,H,DLTA,
     1           TP,TN,NSUBIN,NISQN,DX,LASTI)
C
C ***** FORM NEW P(X) AND CHECK CONVERGENCE ****************
C
      DO 30 I=2,LSTIM1
      IF(DABS(DLTA(I)).GT.CKC*P(I)) JFLAG=1
   30 P(I)=P(I)+DLTA(I)
C
C  ***** CALC. OF IMPROVED N(X) ********************
C
      CALL DELTA(-1.D0,N,NO,DN,DDN,OODN,OODNDT,P,N,C,E,Z,G,H,DLTA,
     1           TP,TN,NSUBIN,NISQN,DX,LASTI)
C
C ***** FORM NEW N(X) AND CHECK CONVERGENCE ****************
C
      DO 32 I=2,LSTIM1
      IF(DABS(DLTA(I)).GT.CKC*N(I)) JFLAG=1
```

```
   32 N(I)=N(I)+DLTA(I)
C
C ***** CALC. OF IMPROVED C(X) ********************
C
      CALL DELTA(Z,C,CO,DC,DDC,0.D0C,OODCDT,P,N,C,E,Z,G,H,DLTA,
     1           TP,TN,NSUBIN,NISQN,DX,LASTI)
C
C ***** FORM NEW C(X) AND CHECK CONVERGENCE ****************
C
      DO 34 I=2,LSTIM1
      IX=I
      CORR=DABS(DLTA(I))
      IF(CORR.LT.DLTSTP.AND.IX.GE.ISTOP) GO TO 35
      IF(CORR.GT.CKC*C(I)) JFLAG=1
   34 C(I)=C(I)+DLTA(I)
   35 ISTOP=IX
      LASTI=ISTOP+10
      IF(LASTI.GT.NP) LASTI=NP
      LSTIM1=LASTI-1
C
C  ************************************************
C
      IF(JFLAG.EQ.1) GO TO 26
C
      INDX=INDX+1
      IF(INDX.EQ.1) GO TO 26
C
      IF(MOD(IT100,IDTPRN).NE.0) GO TO 79
C
      PRINT 213
      PRINT 310,K
      PRINT 304,ITER
      PRINT 312,J
      Y=T/60.DO
      DTN=DT*TNORM
      PRINT 313,T,Y,DTN
```

```
      PRINT 306
C
      XX=DSQRT(4.D0*DSUBC*T)*1.D4
      DO 62 I=1,ISTOP
   62 H(I)=CXE0*DERFC(X(I)/XX)
      ISTOP1=ISTOP+1
   64 DO 66 I=ISTOP1,NP
   66 H(I)=0.D0
C
      DO 69 I=1,N100
      A1=P(I)*CNORM
      A2=N(I)*CNORM
      A3=C(I)*CNORM
      A4=H(I)
      A5=E(I)*ENORM
   69 PRINT 303,I,X(I),A1,A2,A3,A4,A5
   60 DO 70 I=N101,NPM1,N100
      A1=P(I)*CNORM
      A2=N(I)*CNORM
      A3=C(I)*CNORM
      A4=H(I)
      A5=E(I)*ENORM
   70 PRINT 303,I,X(I),A1,A2,A3,A4,A5
C
      A1=P(NP)*CNORM
      A2=N(NP)*CNORM
      A3=C(NP)*CNORM
      A4=0.D0
      A5=E(NP)*ENORM
      PRINT 303,NP,X(NP),A1,A2,A3,A4,A5
C
      PRINT 213
C
      CALL DERIV(E,H,DX,ISTOP)
C
      PRINT 307
```

```
      DO 73 I=1,ISTOP,N100
      A8=H(I)*QNORM
      A9=(P(I)-N(I)+Z*C(I))*QNORM
   73 PRINT 501,I,X(I),A8,A9
C
      PRINT 212
      A15=SIMP(P,DX,NP)*QNORM
      A16=-SIMP(N,DX,NP)*QNORM
      A17=Z*SIMP(C,DX,NP)*QNORM
      A18=A15+A16+A17
      PRINT 502,A15
      PRINT 503,A16
      PRINT 504,A17
      PRINT 505,A18
C
      PRINT 213
      PRINT 402
      PRINT 403
C
      DO 84 I=1,ISTOP,N100
      JPDRI=DSUBP*P(I)*E(I)*JNORM
      JPDIF=-DSUBP*DP(I)*JNORM
      JNDRI=DSUBN*N(I)*E(I)*JNORM
      JNDIF=DSUBN*DN(I)*JNORM
      JCDRI=DSUBC*C(I)*E(I)*JNORM
      JCDIF=-Z*DSUBC*DC(I)*JNORM
      TCUR=JPDRI+JPDIF+JNDRI+JNDIF+JCDRI+JCDIF
   84 PRINT 501,I,X(I),JPDRI,JPDIF,JNDRI,JNDIF,JCDRI,JCDIF,TCUR
C
   79 CONTINUE
C
      IF(MOD(IT100,IDTPUN).NE.0) GO TO 86
C
   85 Y=T/60.D0
      WRITE(7,900) LASTI,Y
      DO 850 I=1,LASTI
```

```
  850 G(I)=C(I)*CNORM
      WRITE(7,901)(G(I),I=1,LASTI)
C
   86 CONTINUE
C
      DO 72 I=1,NP
      CO(I)=C(I)
      EO(I)=E(I)
      NO(I)=N(I)
   72 PO(I)=P(I)
C
   75 GO TO 27
C
  999 CONTINUE
  200 FORMAT(I2)
  201 FORMAT(2X,F8.4,6X,1P7D16.8)
  212 FORMAT(/ )
  213 FORMAT('1')
  250 FORMAT(D10.2)
  301 FORMAT(5D16.8)
  303 FORMAT(1X,I3,F10.5,1P7D17.8)
  304 FORMAT(1X,'TOTAL NO. OF ITERATIONS THUSFAR =',I6/)
  306 FORMAT(6X,'X(MICRONS)',6X,'P(X)',12X,'N(X)',14X,'C(X)',11X,
     1  'CO*ERFC', 9X,'E-FIELD'//)
  307 FORMAT(6X,'X(MICRONS)',5X,'DD/DX',13X,'RHO'//)
  308 FORMAT('1',5X,'BEGINNING OF PART 2, CHANGE OF DELTA X AND DELTA T'
     1//)
  310 FORMAT(1X,'NO. OF TIME STEPS THUSFAR = ',I6/)
  312 FORMAT(1X,'NO. OF ITERATIONS USED IN THIS TIME STEP =',I4/)
  313 FORMAT(1X,'TIME =',F10.2,' SEC. OR',F8.2,' MIN.',5X,'DT =',F5.2,
     1  ' SEC.'//)
  402 FORMAT(////5X,'CURRENT DISTRIBUTION'//)
  403 FORMAT(6X,'X(MICRONS)',3X,'JP(DRIFT)',8X,'JP(DIFF)',9X,'JN(DRIFT)'
     1 ,8X,'JN(DIFF)',9X,'JC(DRIFT)',8X,'JC(DIFF)',9X,'TOTAL J'//)
  406 FORMAT(1X,'THE INTEGRAL OF THE ELECTRIC FIELD = ',1PD16.8)
  501 FORMAT(1X,I3,F10.5,1P7D17.8)
```

```
502 FORMAT(1X,'THE CHARGE DUE TO HOLES = ',1PD16.8,' C/SQ.CM'/)
503 FORMAT(1X,'THE CHARGE DUE TO ELECTRONS = ',1PD16.8,' C/SQ.CM'/)
504 FORMAT(1X,'THE CHARGE DUE TO IMPURITIES = ',1PD16.8,' C/SQ.CM'/)
505 FORMAT(1X,'THE NET CHARGE IN THE MATERIAL = ',1PD16.8,' C/SQ.CM'/)
900 FORMAT(I4,F10.2)
901 FORMAT(1P8E10.3)
    STOP
    END
```

```
      SUBROUTINE FASDER (Y,YSL,YCV,DX,NP)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(1),YSL(1),YCV(1)
      NPM1=NP-1
      NPM2=NP-2
      NPM3=NP-3
      C1=1.D0/(12.D0*DX)
      C2=1.D0/(12.D0*DX*DX)
      DO 300 I=3,NPM2
      YSL(I)=C1*(Y(I-2)-8.D0*(Y(I-1)-Y(I+1))-Y(I+2))
  300 YCV(I)=C2*(-Y(I-2)+16.D0*(Y(I-1)+Y(I+1))-30.D0*Y(I)-Y(I+2))
      C1=1.D0/(2.D0*DX)
      C2=1.D0/(DX*DX)
      DO 400 I=2,NPM1,NPM3
      YSL(I)=C1*(Y(I+1)-Y(I-1))
  400 YCV(I)=C2*(Y(I-1)-2.D0*Y(I)+Y(I+1))
      YSL(1)=(Y(2)-Y(1))/DX
      YSL(NP)=0.D0
      YCV(1)=0.D0
      YCV(NP)=0.D0
      RETURN
      END
```

```
      SUBROUTINE DELTA(ZA,A,AO,DA,DDA,OODA,OODADT,P,N,C,E,Z,G,H,DLTA,
     1                 TP,TN,NSUBIN,NISQN,DX,NP)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 N,NSUBIN,NISQN
      DIMENSION A(1),AO(1),DA(1),DDA(1),P(1),N(1),C(1),E(1),G(1),H(1)
      DIMENSION DLTA(1)
C
      NPM1=NP-1
      NPM2=NP-2
C
C ***** CALC. OF THE COEFFICIENTS G(I) AND H(I) ************
C
      G(1)=0.D0
      H(1)=0.D0
      TODX=2.DO/DX
      TDX=2.D0*DX
C
      DO 100 I=2,NPM1
      ZAEI=ZA*E(I)
C
      RHO=P(I)-N(I)+Z*C(I)
      REC=(N(I)*P(I)-NISQN)/(TP*(N(I)+NSUBIN)+TN*(P(I)+NSUBIN))
C
      AI=TODX+ZAEI
      BI=-((ZA*RHO+A(I)+OODADT)*DX+TODX)*2.D0
      CI=TODX-ZAEI
C
      FCI=TDX*(-DDA(I)+ZAEI*DA(I)+RHO*ZA*A(I)+(A(I)-AO(I))*OODADT+
     1 REC*OODA)
C
      DENI=1.D0/(BI-AI*H(I-1))
      H(I)=CI*DENI
      G(I)=(FCI-AI*G(I-1))*DENI
      IF(DABS(G(I)).LT.1.D-60) G(I)=0.D0
  100 CONTINUE
C
```

```
C ***** CALC. OF THE CORRECTION TERMS **********************
C
      DLTA(NP)=0.D0
      DO 50 I=1,NPM1
      NPMI=NP-I
      DLTA(NPMI)=G(NPMI)-H(NPMI)*DLTA(NPMI+1)
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DERIV(Y,Z,DX,NP)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(1),Z(1)
      NPM1=NP-1
      NPM2=NP-2
      NPM3=NP-3
      C1=1.D0/(12.D0*DX)
      DO 300 I=3,NPM2
  300 Z(I)=C1*(Y(I-2)-8.D0*(Y(I-1)-Y(I+1))-Y(I+2))
      C1=1.D0/(2.D0*DX)
      DO 400 I=2,NPM1,NPM3
  400 Z(I)=C1*(Y(I+1)-Y(I-1))
      Z(1)=(Y(2)-Y(1))/DX
      Z(NP)=(Y(NP)-Y(NPM1))/DX
      RETURN
      END
```

```
      REAL FUNCTION SIMP*8(Y,DX,NP)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(1)
      NPM1=NP-1
      SIMP=(Y(1)+Y(2))*DX/2.D0
      DO 300 I=2,NPM1
  300 SIMP=DX*(-0.5D0*Y(I-1)+4.D0*Y(I)+2.5D0*Y(I+1))/6.D0+SIMP
      RETURN
      END
```

REFERENCES

1. S. Zaromb, "An analysis of diffusion in semiconductors," IBM Journal, pp. 57-61, Jan. 1957.

2. F. M. Smits, "Formation of junction structures by solid-state diffusion," Proc. IRE, pp. 1049-1061, June 1958.

3. A. D. Kurtz and R. Yee, "Diffusion of boron into silicon," Journal of Applied Physics, pp. 303-305, Feb. 1960.

4. K. Lehovec and A Slobodskoy, "Diffusion of charged particles into a semiconductor under consideration of the built-in field," Solid-State Electronics, pp. 45-50, Vol. 3, 1961.

5. D. Shaw and A. L. J. Wells, "The effect of the internal electric field on ionized impurity diffusion in semiconductors," Brit. Journal Applied Physics, pp. 999-1004, vol. 17, 1966.

6. T. Klein and J. R. A. Beal, "Simultaneous diffusion of oppositely charged impurities in semiconductors," Solid-State Electronics, pp. 59-69, Vol. 9, 1966.

7. V. V. Vaskin, V. A. Uskou and M. Ya. Shirobokov, "Effect of the internal electric field on diffusion in semiconductors," Soviet Physics-Solid State, pp. 2703-07, May 1966.

8. N. M. Bordina, A. M. Vasil'ev and D. A. Popov, "Influence of an internal field on diffusion in semiconductors," Soviet Physics-Solid State, pp. 2703-07, May 1966.

9. D. P. Kennedy, "On the ambipolar diffusion of impurities into silicon," Proc. IEEE, pp. 1202-03, June 1969.

10. N. D. Thái, "Concentration-dependent diffusion of boron and phosphorus in silicon," Journal of Applied Physics, pp. 2859-2866, Vol. 41, No.7, June 1970.

11. A. DeMari, "Accurate Numerical Steady-State and Transient One-Dimensional Solutions of Semiconductor Devices," Technical Report, Division of Engineering and Applied Sciences, California Institue of Technology, October, 1967.

12. M. Abramowitz and I. Stegum, ed. Handbook of Mathematical Functions. Washington: U.S. Printing Office, NBS Series no. 55, 1964.

13. F. J. Morin and J. P. Maita, Physics Review, p. 28, Vol. 96, 1954.

14. W. W. Gartner, "Temperature Dependence of Carrier Densities, Mobilities, Diffusion Constants and Conductivities in Germanium and Silicon," Semiconductor Products, pp. 29-31, July, 1960.

15. A. S. Grove, Physics and Technology of Semiconductor Devices. New York: John Wiley and Sons, 1967.

16. A. H. Marshak and D. Assaf III, "A generalized Einstein relation for semiconductors," Solid-State Electronics, in press.

VITA

Ronald Quentin Perritt was born in Deming, New Mexico, on November 30, 1943. In May, 1961, he graduated from Jena High School, Jena, Louisiana. In September, 1961, he entered Louisiana Polytechnic Institute at Ruston, Louisiana; he received his Bachelor of Science degree in Physics in May, 1965. He married Patsy Hagood of Shreveport, Louisiana in August of that year. In September, 1965 he entered the graduate school at Louisiana State University. He subsequently received a Master of Science degree in Electrical Engineering in January, 1968. Mr. Perritt continued his graduate work at Louisiana State University and is presently a candidate for the Doctor of Philosophy degree in Electrical Engineering. During most of the past four years he has served as an instructor in the Electrical Engineering Department.

EXAMINATION AND THESIS REPORT

Candidate: Ronald Quentin Perritt

Major Field: Electrical Engineering

Title of Thesis: A Numerical Study of Field-Aided Diffusion

Approved:

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

Date of Examination:

December 4, 1972